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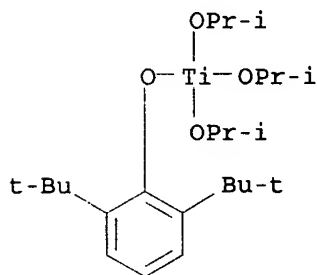
ANSWER 1 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:34577 CAPLUS  
 DOCUMENT NUMBER: 142:114681  
 TITLE: Titanium alkoxide catalysts for polymerization of cyclic esters and methods of polymerization  
 INVENTOR(S): Verkade, John G.; Kindel, Jnaneshwara Ganesh  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 43 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005009687	A1	20050113	US 2004-837257	20040430
PRIORITY APPLN. INFO.:			US 2003-467435P	P 20030502

AB Titanium alkoxide catalysts for polymerization of cyclic esters such as lactide (LA) and caprolactone (CL) and methods of polymerization are disclosed. Titanium is known to be non-toxic and the various compds. described herein can catalyze cyclic esters to produce polyesters with controlled mol. wts. and relatively narrow mol. weight distributions. In one embodiment, caged titanium alkoxides catalysts are used. The caged titanium alkoxides can be atranes or non-atranes.

IT 821008-91-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; titanium alkoxide catalysts for polymerization of cyclic esters and methods of polymerization)

RN 821008-91-7 CAPLUS  
 CN INDEX NAME NOT YET ASSIGNED



L6 ANSWER 2 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:672996 CAPLUS  
 DOCUMENT NUMBER: 141:359848  
 TITLE: Synthesis and Characterization of a Series of Rubidium Alkoxides and Rubidium-Titanium Double Alkoxides  
 AUTHOR(S): Bunge, Scott D.; Boyle, Timothy J.; Pratt, Harry D., III; Alam, Todd M.; Rodriguez, Mark A.  
 CORPORATE SOURCE: Sandia National Laboratories, Advanced Materials Laboratory, Albuquerque, NM, 87106, USA  
 SOURCE: Inorganic Chemistry (2004), 43(19), 6035-6041  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB This report studies the structural aspects of the products isolated from the reactions of Ti alkoxides { [Ti(OR)<sub>4</sub>]<sub>n</sub> n = 2, OR = OCH<sub>2</sub>CMe<sub>3</sub>

(ONep) (1);  $n = 1$ ,  $\text{OC}_6\text{H}_3\text{Me}_2$ -2,6 (DMP) (2)} with Rb alkoxides  $\{[\text{Rb}(\text{OR})]_\infty$  where  $\text{OR} = (\text{ONep})$  (3), (DMP) (4), and  $\text{OC}_6\text{H}_3(\text{CHMe}_2)_2$ -2,6 (DIP) (5)}. The resultant double alkoxides were determined by single crystal x-ray diffraction to be  $[\text{Rb}(\mu\text{-ONep})_4(\text{py})\text{Ti}(\text{ONep})]_2$  (6),  $[\text{Rb}(\mu\text{-DMP})\text{Ti}(\text{DMP})_4]_\infty$  (7), and  $[\text{Rb}(\mu\text{-DMP})_2(\mu\text{-ONep})_2\text{Ti}(\text{ONep})]_\infty$  (8). Compound 1 is the previously reported dinuclear species with trigonal bipyramidal Ti metal centers whereas compound 2 is a monomer with a tetrahedral Ti center. Suitable x-ray quality crystals of 3 were not isolated. Compds. 4 and 5 demonstrate extended polymeric networks with Rb coordination ranging from two to five using terminal  $\mu$ - and  $\mu_3$ -OR ligands and  $\pi$ -interactions of neighboring OAr ligands. The double alkoxide 6 revealed a simple tetranuclear structure with  $\mu$ -ONep acting as the bridge, terminal ONep ligands on the Ti, and one terminal py on the Rb. For 7 and 8, the  $\pi$ -interaction facilitated the formation of extended polymeric systems. All complexes were further characterized by FTIR and multinuclear NMR spectroscopy.

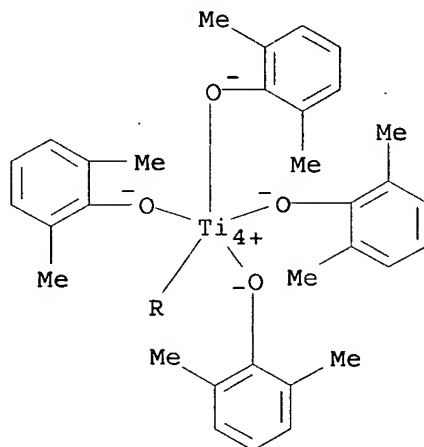
IT 776299-09-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymeric; preparation and crystal structure of)

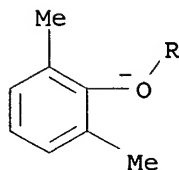
RN 776299-09-3 CAPLUS

CN Titanate(1-), pentakis(2,6-dimethylphenolato)-, rubidium, (TB-5-11)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



● Rb<sup>+</sup>

REFERENCE COUNT:

44

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:621164 CAPLUS

DOCUMENT NUMBER: 141:288262

TITLE: Simultaneous determination of phenylglycidol enantiomers and cinnamyl alcohol in asymmetric epoxidation processes by chiral liquid chromatography

AUTHOR(S): Morante-Zarcelero, Sonia; Perez, Yolanda; del Hierro, Isabel; Fajardo, Mariano; Sierra, Isabel

CORPORATE SOURCE: E.S.C.E.T., Departamento de Tecnologia Quimica, Ambiental y de los Materiales, Universidad Rey Juan Carlos, Madrid, 28933, Spain

SOURCE: Journal of Chromatography, A (2004), 1046(1-2), 61-66  
CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A HPLC method was developed for the simultaneous determination of phenylglycidol

enantiomers and cinnamyl alc. (CA). Sepns. were achieved on an amylose tris(3,5-dimethylphenylcarbamate) chiral stationary phase (Chiralpak AD). The effect of concentration of organic modifier (2-propanol and ethanol) in the mobile phase and flow-rate was studied. The mobile phase selected consisted of a mixture of n-hexane-ethanol (85:15, volume/volume) with a flow-rate of 1.2 mL/min. The UV-visible detector was set at 254 nm. Resolution for the phenylglycidol enantiomers in the suitable chromatog. conditions was 2.4 with an anal. time of 12 min. The method developed was validated and is linear at  $5 + 10^{-4}$  -  $3 + 10^{-2}$  M, for phenylglycidol enantiomers and at  $5 + 10^{-5}$  -  $1 + 10^{-3}$  M, for CA ( $r > 0.999$  for the three compds.). Repeatability and intermediate precision for the three analytes at three different concns. were  $<3.6$  and  $2.8\%$  relative standard deviation, resp. This method was applied to study the asym. epoxidn. of CA with titanium(IV) alkoxide compds. as catalysts to evaluate their catalytic activity and stereoselectivity of the epoxidn. processes.

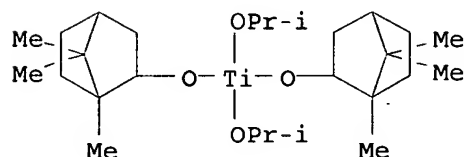
IT 374567-07-4

RL: CAT (Catalyst use); USES (Uses)

(catalyst; simultaneous determination of phenylglycidol enantiomers and cinnamyl alc. in catalytic asym. epoxidn. processes by chiral liquid chromatog.)

RN 374567-07-4 CAPLUS

CN Titanium, bis(2-propanolato)bis[(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-olato]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:612104 CAPLUS

DOCUMENT NUMBER: 141:140911

TITLE: Manufacture of (meth)acrylic acid esters with cyclic secondary or tertiary alcohols

INVENTOR(S): Kenmochi, Hiroyuki; Hori, Yoji; Hasegawa, Yoshiki

PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004210745	A2	20040729	JP 2003-2449	20030108
PRIORITY APPLN. INFO.: .			JP 2003-2449	20030108

OTHER SOURCE(S): MARPAT 141:140911

AB The esters are manufactured by reaction of H<sub>2</sub>C:CR<sub>1</sub>CO<sub>2</sub>A (R<sub>1</sub> = H, Me; A = COR<sub>2</sub>, SO<sub>2</sub>R<sub>3</sub>, POR<sub>4</sub>; R<sub>2</sub> = tert-Bu, 2,3-dimethyl-2-Bu, 2-methyl-2-pentyl, 3-methyl-3-pentyl, 4-nitrophenyl, 2,4,6-trichlorophenyl; R<sub>3</sub> = Me, Ph, p-tolyl, CF<sub>3</sub>; R<sub>4</sub> = MeO, EtO, PrO, Me<sub>2</sub>CHO, PhO) with cyclic secondary or tertiary alcs. selected from alicyclic alc. metal alkoxides, hydroxylactones, and condensed alicyclic lactone ring-containing alcs. Thus, acrylic acid was treated with equimolar 2,2-dimethylpropionyl chloride in PhMe in the presence of Et<sub>3</sub>N, washed, mixed with hydroquinone monomethyl ether, freed of PhMe, and evaporated to give an acrylic acid-2,2-dimethylpropionic acid mixed anhydride (I; purity 67.6%). THF containing 15.0 g 2-adamantanone and 11.78 g iso-Pr chloride was added dropwise to THF containing Li, stirred at 20° for 5 h, solvent-substituted by PhMe, treated with 25.2 g I, washed, freed of solvent, mixed with hydroquinone monomethyl ether, and evaporated to give 61.4% 2-isopropyl-2-adamantyl acrylate.

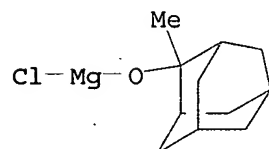
IT 725404-08-0P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of (meth)acrylic acid esters with cyclic alcs. by using mixed anhydrides)

RN 725404-08-0 CAPLUS

CN Magnesium, chloro(2-methyltricyclo[3.3.1.1<sup>3,7</sup>]decan-2-olato)- (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:515582 CAPLUS

DOCUMENT NUMBER: 141:72041

TITLE: Ring-opening polymerization reaction and metal complex catalyst therefor

INVENTOR(S): Partridge, Martin Graham; Davidson, Matthew Gwilym; Eade, Gillian Frances

PATENT ASSIGNEE(S): Johnson Matthey Plc, UK

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052980	A1	20040624	WO 2003-GB5386	20031210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				

GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,  
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,  
 OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,  
 TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,  
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

GB 2002-28888

A 20021211

OTHER SOURCE(S): MARPAT 141:72041

AB The invention provides a compound suitable for use as a catalyst for ring opening polymerization reactions for example for the polymerization of lactones,

lactides etc., the catalyst comprising the reaction product of (i) an alkoxide, halide, condensed alkoxide, amide, condensed amide, mixed halo-alkoxide or, mixed halo-amide, sulfonic acid derivative, sulfonamide, silanol or silylamide of titanium zirconium, hafnium or aluminum or a mixture thereof, and (ii) a complexing compound selected from the list comprising oximes, hydroxy-Schiff bases, 8-hydroxyquinoline derivs., 10-hydroxybenzo-[h]-quinoline derivs., hydrazones and substituted phenols.  $\text{Ti}(\text{O-iso-Pr})_3(\eta^2\text{-OC}_6\text{H}_2\text{Cl}_2\text{CHN}(\text{C}_6(\text{CMe}_3)_3\text{H}_2))$  was prepared and used to polymerize caprolactone.

IT 500571-21-1P 500571-23-3P 500571-28-8P

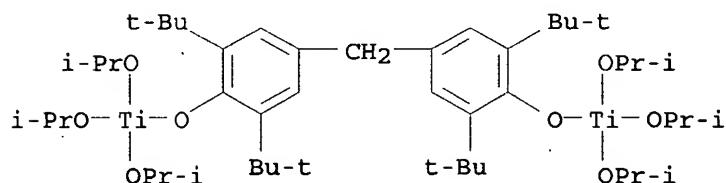
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);

USES (Uses)

(ring-opening polymerization reaction and metal complex catalyst therefor)

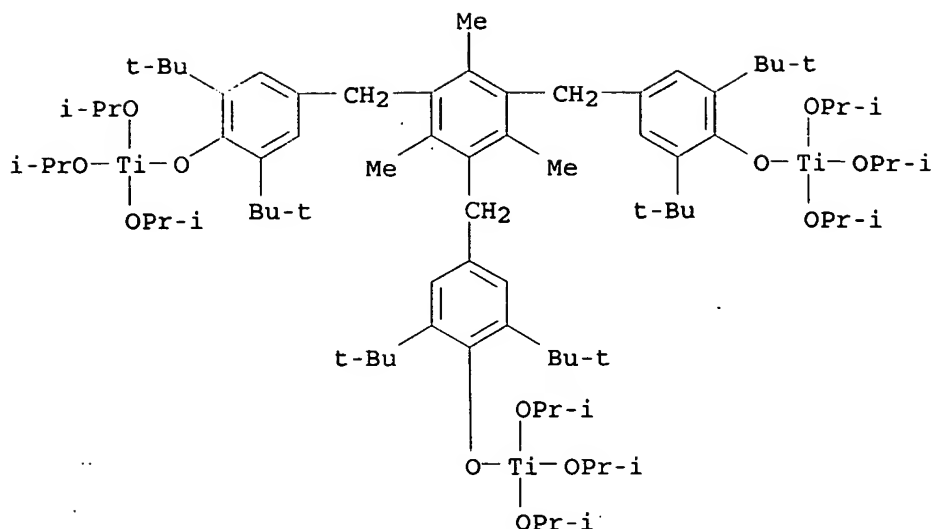
RN 500571-21-1 CAPLUS

CN Titanium,  $[\mu\text{-}[[4,4'\text{-methylenebis}(2,6\text{-bis}(1,1\text{-dimethylethyl})\text{phenolato-}\kappa\text{O})](2\text{-})]]\text{hexakis}(2\text{-propanolato})\text{di-}$  (9CI) (CA INDEX NAME)

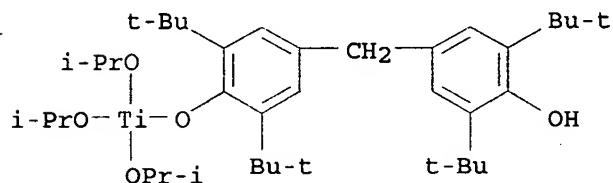


RN 500571-23-3 CAPLUS

CN Titanium, nonakis(2-propanolato)  $[\mu_3\text{-}[[4,4',4''\text{-}[(2,4,6\text{-trimethyl-1,3,5-benzenetriyl})\text{tris(methylene)}]\text{tris}(2,6\text{-bis}(1,1\text{-dimethylethyl})\text{phenolato-}\kappa\text{O})](3\text{-})]]\text{tri-}$  (9CI) (CA INDEX NAME)



RN 500571-28-8 CAPLUS  
 CN Titanium, [4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-2,6-bis(1,1-dimethylethyl)phenolato-κO]tris(2-propanolato)-, (T-4)-(9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2004:268541 CAPLUS  
 DOCUMENT NUMBER: 140:303849  
 TITLE: Regioselective preparation of β-substituted silyl enolates and ketones via titanium enolates from α,β-unsaturated ketones  
 INVENTOR(S): Hayashi, Tamio  
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004099524	A2	20040402	JP 2002-263698	20020910
PRIORITY APPLN. INFO.:			JP 2002-263698	20020910
OTHER SOURCE(S): MARPAT 140:303849				

AB The silyl enolates X<sub>3</sub>SiOCR<sub>1</sub>:CHCHR<sub>2</sub>R<sub>3</sub> [R<sub>1</sub>, R<sub>2</sub> = [halo-, C<sub>1</sub>-10 (un)saturated aliphatic hydrocarbyl-, C<sub>6</sub>-14 aryl-, etc. substituted] C<sub>1</sub>-10 alkyl; R<sub>1</sub> and R<sub>2</sub> may form ring; R<sub>3</sub> = [halo-, C<sub>1</sub>-10 (un)saturated aliphatic hydrocarbyl-, C<sub>6</sub>-14 aryl-, etc. substituted] C<sub>6</sub>-14 aryl; X = C<sub>1</sub>-10 alkyl, Ph] are prepared by reaction of R<sub>1</sub>C(O)C:CHR<sub>2</sub> (R<sub>1</sub>, R<sub>2</sub> = same as above) with R<sub>3</sub>TiY<sub>3</sub> (R<sub>3</sub> = same as above; Y = C<sub>1</sub>-6 alkoxy) in the presence of Rh catalysts and reaction of the resulting Y<sub>3</sub>TiOCR<sub>1</sub>:CHCHR<sub>2</sub>R<sub>3</sub> (I; R<sub>1</sub>-R<sub>3</sub>, Y = same as above) with silyl

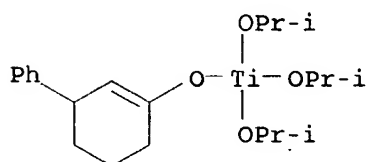
compds. and metal alkoxides. The ketones R1C(O)CH2CHR2R3 (R1-R3 = same as above) are prepared by treatment of I (R1-R3, Y = same as above) with protic polar solvents. Optically active enolates and ketones may be prepared by using optically active Rh catalysts. PhTi(OPr-iso)3 was treated with 2-cyclohexenone in the presence of [Ph(OH)((S)-binap)]2 in THF at 20° for 1 h and treated with LiOPr-iso and Me3SiCl at room temperature for 1 h to give 84% (S)-3-phenyl-1-trimethylsiloxy cyclohex-1-ene with 99.5% e.e.

IT 676270-00-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(regioselective preparation of Ti enolates by treatment of  $\alpha,\beta$ -unsatd. ketones with organotitanium compds. in the presence of Rh catalysts)

RN 676270-00-1 CAPLUS

CN Titanium, (3-phenyl-1-cyclohexen-1-olato)tris(2-propanolato)-, (T-4)-(9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:173677 CAPLUS

DOCUMENT NUMBER: 138:205485

TITLE: Metal complex polymerization catalysts, their manufacture and curable compositions

INVENTOR(S): Davidson, Matthew Gwilym; Lunn, Matthew David Gwydion; Johnson, Andrew Lee; Stengel, Bruno Frederic

PATENT ASSIGNEE(S): Johnson Matthey Plc, UK

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003018662	A1	20030306	WO 2002-GB3896	20020823
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: GB 2001-20743 A 20010825

OTHER SOURCE(S): MARPAT 138:205485

AB A compound suitable for use as a catalyst for the formation of urethanes and ureas comprises the reaction product of (i) an alkoxide, condensed alkoxide or halo-alkoxide of Ti Zr, Hf or Al or a mixture, and (ii) a complexing compound selected from oximes, hydroxy Schiff bases, 8-hydroxyquinoline derivs., 10-hydroxybenzo-[h]-quinoline

derivs., hydrazones and substituted phenols. Thus, an example catalyst hexa(salicylaldominato)tetraisopropoxy titanate (preparation given) had m.p. 145-147°.

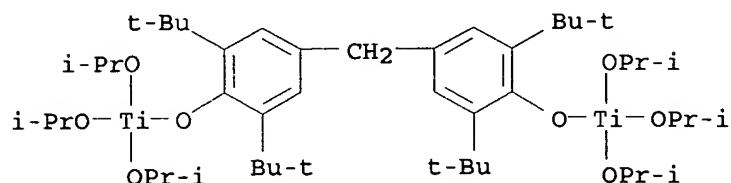
IT 500571-21-1P 500571-23-3P 500571-28-8P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(catalysts for reactions forming urethanes, ureas, and epoxy resins)

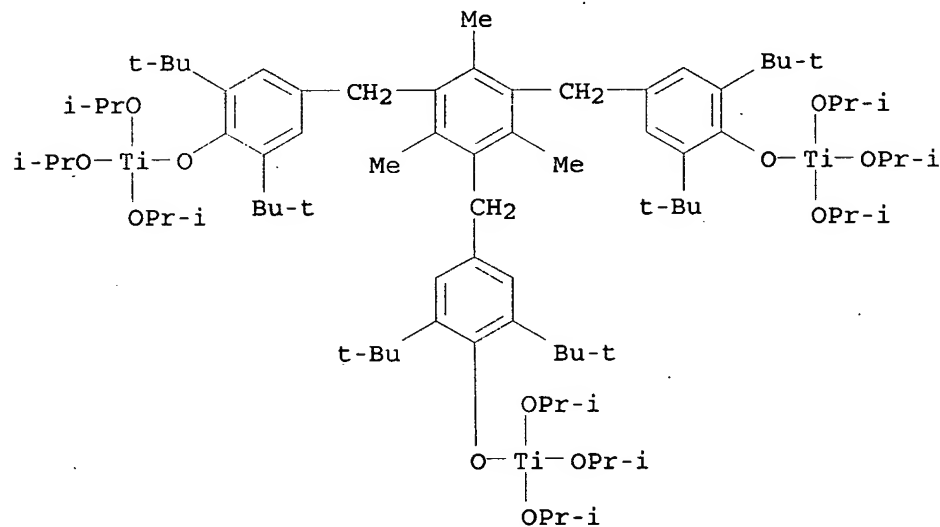
RN 500571-21-1 CAPLUS

CN Titanium, [ $\mu$ -[[4,4'-methylenebis[2,6-bis(1,1-dimethylethyl)phenolato- $\kappa$ O]](2-)]hexakis(2-propanolato)di- (9CI) (CA INDEX NAME)



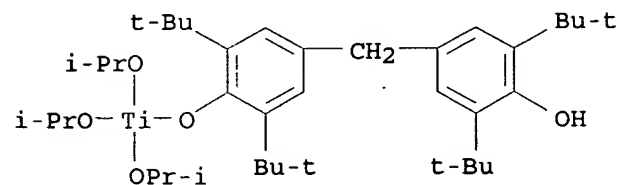
RN 500571-23-3 CAPLUS

CN Titanium, nonakis(2-propanolato)[ $\mu$ 3-[[4,4',4''-(2,4,6-trimethyl-1,3,5-benzenetriyl)tris(methylene)]tris[2,6-bis(1,1-dimethylethyl)phenolato- $\kappa$ O]](3-)]tri- (9CI) (CA INDEX NAME)



RN 500571-28-8 CAPLUS

CN Titanium, [4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]-2,6-bis(1,1-dimethylethyl)phenolato- $\kappa$ O]tris(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)





L6 ANSWER 8 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:126117 CAPLUS

DOCUMENT NUMBER: 138:402127

TITLE: Binolate complexes of lithium, zinc, aluminium, and titanium; preparations, structures, and studies of lactide polymerization

AUTHOR(S): Chisholm, Malcolm H.; Lin, Chu-Chieh; Gallucci, Judith C.; Ko, Bao-Tsan

CORPORATE SOURCE: Newman and Wolfrom Laboratories, Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA

SOURCE: Dalton Transactions (2003), (3), 406-412

CODEN: DTARAF; ISSN: 1477-9226

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of racemic 5,5',6,6'-tetramethyl-3,3'-di-tert-butyl-1,1'-biphenyl-2,2'-diol (biphenolate-H<sub>2</sub>) with 4 mol equivalent of nBuLi yields [(μ<sub>3</sub>,μ<sub>3</sub>-biphenolate)<sub>2</sub>Li<sub>4</sub>(nBuLi)<sub>4</sub>] (1) in high yield. 1 Further reacts with 4 mol equivalent of 2,4-dimethyl-3-pentanol in the presence of THF or cyclohexene oxide (CyHO) to give the lithium aggregate [(μ,μ-biphenolate)Li<sub>2</sub>(μ<sub>3</sub>-OCH(iPr)<sub>2</sub>)<sub>2</sub>Li<sub>2</sub>(L)<sub>2</sub>] (2-THF, L = THF; 2-CyHO, L = CyHO). Treatment of biphenolate-H<sub>2</sub> with 3 mol equivalent of ZnEt<sub>2</sub>, followed by addition of 2 mol equivalent of 2,4-dimethyl-3-pentanol provides the zinc complex [(μ,μ-biphenolate)Zn(μ-OCH(iPr)<sub>2</sub>)<sub>2</sub>Zn<sub>2</sub>Et<sub>2</sub>] (3). Aluminum alkoxide incorporating biphenolate ligand can also be obtained via a similar synthetic route. The compound [(μ-biphenolate)AlMe(μ-OCH(iPr)<sub>2</sub>)AlMe<sub>2</sub>] (4) is prepared from the reaction of biphenolate-H<sub>2</sub> with 2 mol equivalent of AlMe<sub>3</sub> in the presence of 1 mol equivalent of 2,4-dimethyl-3-pentanol. The titanium (4+) binolate complex [(biphenolate)Ti<sub>2</sub>Cl<sub>6</sub>] (5) is synthesized from the reaction of biphenolate-H<sub>2</sub> and 2 mol equivalent of TiCl<sub>4</sub>. In addition, 2-THF,

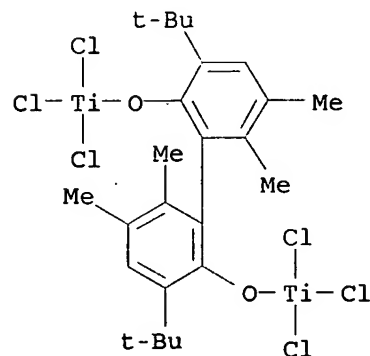
3, and 4 have been examined for rac-lactide polymerization, and the comparative studies of polymerization are also presented.

IT 529487-73-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation of binolate metal complexes for lactide polymerization)

RN 529487-73-8 CAPLUS

CN Titanium, [μ-[3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diolato(2-)-κO:κO']]hexachlorodi- (9CI) (CA INDEX NAME)



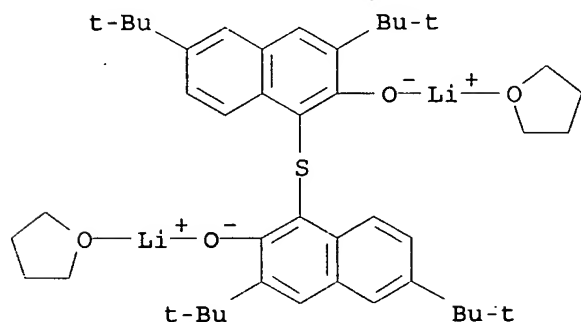
REFERENCE COUNT:

36

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:175920 CAPLUS  
DOCUMENT NUMBER: 137:102896  
TITLE: Symmetric and asymmetric samarium alkoxide derivatives of bridging sulfur biphenolate and binaphtholate ligands; synthetic, structural, and catalytic studies  
AUTHOR(S): Arnold, Polly L.; Natrajan, Louise S.; Hall, Jonathan J.; Bird, Stephan J.; Wilson, Claire  
CORPORATE SOURCE: School of Chemistry, University of Nottingham, Nottingham, NG7 2RD, UK  
SOURCE: Journal of Organometallic Chemistry (2002), 647(1-2), 205-215  
CODEN: JORCAI; ISSN: 0022-328X  
PUBLISHER: Elsevier Science B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:102896  
AB The new thio-binaphthol 1,1'-thiobis(3,6-di-tert-butyl-naphth-2-ol), and the phenolic analog 1,1'-thiobis(6-tert-butyl-4-methylphen-2-ol) react with the Sm(III) aryloxide [Sm(OC<sub>6</sub>H<sub>3</sub>But<sub>2</sub>-2,6)<sub>3</sub>] to give the 1st f-element complexes supported by S-bridged biphenolate or binaphtholate ancillary ligands, [Sm{1,1'-S(2-OC<sub>10</sub>H<sub>4</sub>But<sub>2</sub>-3,6)<sub>2</sub>}(OC<sub>6</sub>H<sub>3</sub>But<sub>2</sub>-2,6)]<sub>2</sub> and [Sm{1,1'-S(2-OC<sub>6</sub>H<sub>2</sub>But-3-Me-5)<sub>2</sub>}(OC<sub>6</sub>H<sub>3</sub>But<sub>2</sub>-2,6)]<sub>2</sub>. Sym. and asym. derivs. of both ligands were prepared by careful tuning of the preparative procedure. The asym. naphtholate derivative, and the ligand from which it derives have both been structurally characterized. The asym. derivs. are highly selective catalysts for diol desymmetrization.  
IT 442199-66-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(reactant for preparation of samarium(III) di-tert-butylphenolate thiobis(di-tert-butyl-naphthol) complex)  
RN 442199-66-8 CAPLUS  
CN Lithium, bis(tetrahydrofuran) [[1,1'-thiobis[3,6-bis(1,1-dimethylethyl)-2-naphthalenolato-κO]](2-)]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:159172 CAPLUS  
DOCUMENT NUMBER: 136:349718  
TITLE: Radical Scission of Symmetrical 1,4-Dicarbonyl Compounds: C-C Bond Cleavage with Titanium(IV) Enolate Formation and Related Reactions  
AUTHOR(S): Agapie, Theodor; Diaconescu, Paula L.; Mindiola, Daniel J.; Cummins, Christopher C.  
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of

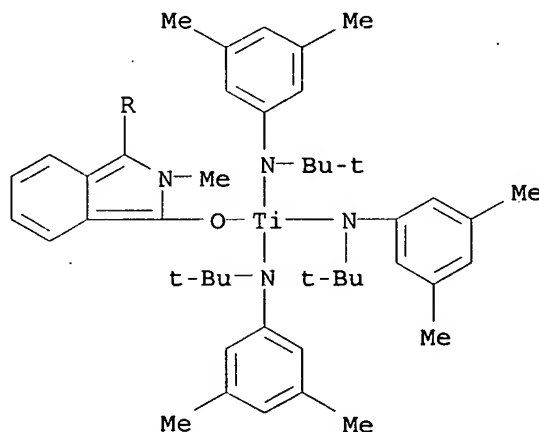
SOURCE: Technology, Cambridge, MA, 02139-4307, USA  
 Organometallics (2002), 21(7), 1329-1340  
 CODEN: ORGND7; ISSN: 0276-7333  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:349718

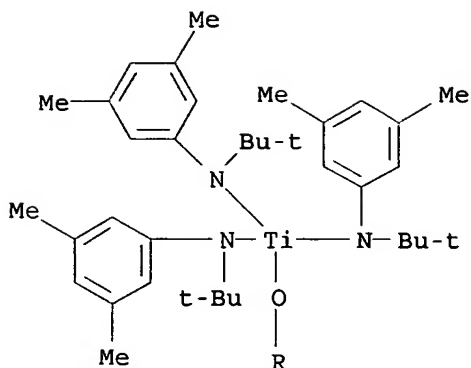
AB Reaction of  $\text{Ti}(\text{NRAr1})_3$  (1, R = CMe<sub>3</sub>, Ar1 = 3,5-C<sub>6</sub>H<sub>3</sub>Me<sub>2</sub>) with 0.5 equiv of sym. 1,4-diketones ( $\text{ArCOCH}_2$ )<sub>2</sub> (Ar = p-Tol or p-MeOC<sub>6</sub>H<sub>4</sub>) in hydrocarbon solvents at  $\leq 25^\circ$  resulted in carbon-carbon bond cleavage with clean formation of titanium-bound enolates, 1-OC(CH<sub>2</sub>)Ar. Treatment of  $\text{Ti}(\text{NRAr1})_3$  with esters or amides of succinic acid, under the same mild conditions, smoothly produced titanium(IV) compds. containing the corresponding amide or ester enolate moiety. The amide enolate condenses with benzaldehyde in an aldolic fashion. Differences in the observed reactivity of amido-enolate vs. ketone-derived enolate toward aldol condensation were interpreted with the help of computational methods. Upon reaction with  $\text{Ti}(\text{NRAr1})_3$ , para-substituted acetophenones yielded equal amts. of enolate and alkoxide products. Under similar exptl. conditions, acetophenone itself produced quant. a species whose proposed structure incorporates characteristics reminiscent of a Gomberg dimer. This intermediate decompd. cleanly to the expected enolate and alkoxide mixture upon heating.  $\text{Ti}(\text{NRAr1})_3$  reductively complexes substrates such as N-Me phthalimide. Treatment of  $\text{Ti}(\text{NRAr1})_3$  with 0.5 equiv of o-bromophenyl allyl ether resulted in bromine atom abstraction followed by cyclization of the intermediate aryl radical to generate a titanium-bound 3-methylenedihydrobenzofuran product.

IT 417710-18-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation from reaction of titanium(III) xylyl(butyl)amide complex with methylphthalimide)

RN 417710-18-0 CAPLUS  
 CN Titanium, hexakis[N-(1,1-dimethylethyl)-3,5-dimethylbenzenamato] [ $\mu$ -[2-methyl-2H-isoindole-1,3-diolato(2-)- $\kappa\text{O1}:\kappa\text{O3}$ ]]di- (9CI) (CA INDEX NAME)

PAGE 1-A





REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:667354 CAPLUS

DOCUMENT NUMBER: 135:380208

TITLE: Achiral Tetrahydrosalen Ligands for the Synthesis of C2-Symmetric Titanium Complexes: A Structure and Diastereoselectivity Study

AUTHOR(S): Balsells, Jaume; Carroll, Patrick J.; Walsh, Patrick J.

CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA

SOURCE: Inorganic Chemistry (2001), 40(22), 5568-5574

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:380208

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Achiral tetrahydrosalen ligands were employed in the synthesis of chiral C2-sym. Ti complexes. When combined with tetrahydrosalen ligands 2a (I) and 2b (II), Ti tetraisopropoxide liberated 2 equiv of iso-Pr alc. and generated the (tetrahydrosalen)Ti(O-i-Pr)<sub>2</sub> complexes 3a and 3b. These complexes are C2-sym. by <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>H} NMR spectrometry and x-ray crystallog. x-ray structures of 3a and 3b indicate that the bonding of the tetrahydrosalen ligand to Ti is different than the bonding of salen ligands to Ti. Whereas salen ligands usually bind to Ti in a planar arrangement, the tetrahydrosalen is bonded with the phenoxide oxygens mutually trans. When bound in this fashion, the nitrogens of the tetrahydrosalen ligand and the Ti become stereogenic centers. The use of Ti complexes of high enantiopurity in the generation of tetrahydrosalen Ti adducts resulted in a maximum diastereoselectivity of 2:1. The diastereoselectivity obtained using chiral Ti alkoxide complexes was greater than the diastereoselectivity observed when a tetrahydrosalen ligand derived from (S,S)-trans-diaminocyclohexane was employed.

IT 374567-07-4

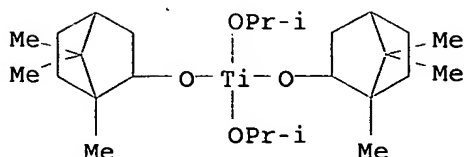
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with bis(hydroxyphenylmethyl)ethylenediamine derivs.)

RN 374567-07-4 CAPLUS

CN Titanium, bis(2-propanolato)bis[(1S,2R,4S)-1,7,7-

trimethylbicyclo[2.2.1]heptan-2-olato]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:535185 CAPLUS

DOCUMENT NUMBER: 133:120817

TITLE: Metallocene catalyst compositions for manufacture of syndiotactic polystyrene homopolymers and copolymers

INVENTOR(S): Yabunouchi, Nobuhiro; Tomotsu, Norio

PATENT ASSIGNEE(S): Idemitsu Petrochemical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044794	A1	20000803	WO 2000-JP230	20000119
W: JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1085026	A1	20010321	EP 2000-900822	20000119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6825294	B1	20041130	US 2000-646128	20000928
PRIORITY APPLN. INFO.:			JP 1999-22076	A 19990129
			WO 2000-JP230	W 20000119

OTHER SOURCE(S): MARPAT 133:120817

AB The compns. efficiently and inexpensively producing syndiotactic polystyrenes comprise: (A) a transition metal compound, (B) O-containing compound

or/and compound which can form ionic complex with the A, (C) an organometallic compound, preferably an organoaluminum compound of formula: [(R1)3CO]nAl(R2)3-n (wherein R1 = C1-30 aliphatic hydrocarbyl group, C6-30 aromatic hydrocarbyl group, etc.; R2 = hydrocarbyl group; n = 1, 2), and (D) an alkylating agent if needed. Thus, mixing 23.9 mL MePh with 0.38 mL a 2 mol/L solution of iso-Bu3Al in MePh, 1.05 mL a 1.43 mol/L solution of Me aluminoxane in MePh, and 0.12 mL a 250 mmol/L solution of 1,2,3,4,5,6,7,8-octahydrofluorenyltitanium trimethoxide in MePh gave a catalyst mixture, 1.25 mL of which was combined with 50 mL of styrene and 0.20 mL of a 0.1 mol/L solution of diisobutyl(triphenylmethoxy)aluminum in MePh and polymerized at 70° for 1 h to give a syndiotactic polystyrene with weight-average mol. weight of 420,000 and catalyst activity of 412 kg/g-Ti.

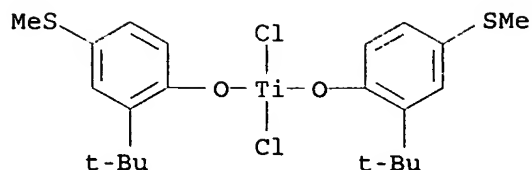
IT 286015-48-3

RL: CAT (Catalyst use); USES (Uses)

(polymerization catalyst; metallocene catalyst compns. for manufacture of syndiotactic polystyrene homopolymers and copolymers)

RN 286015-48-3 CAPLUS

CN Titanium, dichlorobis[2-(1,1-dimethylethyl)-4-(methylthio)phenolato-κO]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:535184 CAPLUS

DOCUMENT NUMBER: 133:151078

TITLE: Metallocene catalyst compositions for olefin polymerizations and copolymerizations

INVENTOR(S): Yabunouchi, Nobuhiro; Minami, Yutaka; Tomotsu, Norio

PATENT ASSIGNEE(S): Idemitsu Petrochemical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 88 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044793	A1	20000803	WO 2000-JP229	20000119
W: CA, JP, KR, SG, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1157393	A1	20020102	EP 2000-900821	20000119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRIORITY APPLN. INFO.:		JP 1999-22075	A	19990129
		JP 1999-146305	A	19990526
		WO 2000-JP229	W	20000119

OTHER SOURCE(S): MARPAT 133:151078

AB The compns. with high activity and reduced amount of co-catalyst, e.g., an O-containing compound which can manufacture polyolefins efficiently and at low cost

comprise: (A) a transition metal compound, (B) an O-containing compound or a compound capable of forming an ionic complex with A, (C) an organometallic compound, preferably an organoaluminum compound, such as a reaction product (I) of triphenylmethanol with triisobutylaluminum and (D) optionally an alkylating agent. Thus, preparing a compound I and a silica-supported Me aluminosilane (II), mixing 50  $\mu$ mol. I and 0.25 mmol (as Al atom) II with 0.5 mmol iso-Bu<sub>3</sub>Al and 1  $\mu$ mol dimethylsilylenebis(2-methyl-4,5-benzoinderyl)zirconium dichloride in MePh in a reactor, compressing with propylene gas to 0.785 MPa-gage, and polymerizing at 70° for 60 min gave 33.2 g polypropylene with weight-average mol. weight of 1,070,000, mol.-weight distribution 2.07 and stereospecificity of 97.2%.

IT 286015-48-3

RL: CAT (Catalyst use); USES (Uses)

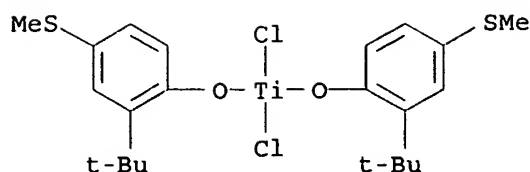
(polymerization catalyst; metallocene catalyst compns. for olefin polymns.

and

copolymns.)

RN 286015-48-3 CAPLUS

CN Titanium, dichlorobis[2-(1,1-dimethylethyl)-4-(methylthio)phenolato- $\kappa$ O]-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:600900 CAPLUS

DOCUMENT NUMBER: 131:251717

TITLE: Soluble complexes of  $[\text{FeH}_6]^{4-}$

AUTHOR(S): Linn, Donald E., Jr.; Skidd, Gabriel M.; Tippmann, Eric M.

CORPORATE SOURCE: Department of Chemistry, Indiana University-Purdue University Fort Wayne, Fort Wayne, IN, 46805-1499, USA

SOURCE: Inorganica Chimica Acta (1999), 291(1-2), 142-147  
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An improved laboratory bench top solution synthesis of the complex hydride, hexahydridoferate ion,  $[\text{FeH}_6]^{4-}$ , is reported giving > 40% yield. The reaction involves the hydrogenation of a mixture of Fe(II) halide and phenylmagnesium halide at room temperature and 4.4 bar  $\text{H}_2$  pressure. The product,  $[\text{FeH}_6][\text{MgBr}(\text{THF})_2]_4$  is only moderately soluble in THF and ppts. as a yellow powder. and is conveniently characterized by  $^1\text{H}$  NMR, IR and UV-visible spectroscopy. The moderate solubility of the above complex

containing

the  $[\text{Mg}(\text{THF})_n]^+$  counterion is markedly improved by substitution of the bromide with an alkoxide. The complexes containing  $[\text{MgOR}(\text{THF})_n]^+$  are readily soluble in ether and aromatic hydrocarbons such as benzene. A limited number of H transfer reactions showed that  $[\text{FeH}_6]^{4-}$ , has potential as a stoichiometric and catalytic multiple H-transfer agent.

IT 244247-12-9P

RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);

PREP (Preparation); USES (Uses)

(preparation, IR and NMR spectra, and hydrogen transfer catalyst for hydrogen transfer and hydrogenation of p-xylene)

RN 244247-12-9 CAPLUS

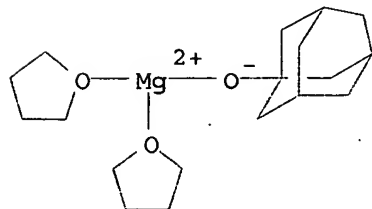
CN Magnesium(1+), bis(tetrahydrofuran)(tricyclo[3.3.1.1<sup>3,7</sup>]decan-1-olato)-, (OC-6-11)-hexahydroferrate(4-) (4:1) (9CI) (CA INDEX NAME)

CM 1

CRN 244247-11-8

CMF C18 H31 Mg O3

CCI CCS

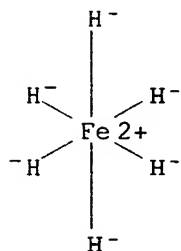


CM 2

CRN 91208-66-1

CMF Fe H6

CCI CCS



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:287646 CAPLUS

DOCUMENT NUMBER: 128:303308

TITLE: Complexes of Strong Bidentate Lewis Acids Derived from 2,7-Bis(1,1-dimethylethyl)fluorene-1,8-diol

AUTHOR(S): Saied, Okba; Simard, Michel; Wuest, James D.

CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.

SOURCE: Inorganic Chemistry (1998), 37(11), 2620-2625

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Treatment of 2,7-bis(1,1-dimethylethyl)fluorene-1,8-diol (3) with 2 equiv of  $\text{TiCl}_4$  converts the two OH groups into  $\text{OTiCl}_3$  groups and thereby yields bis(trichlorotitanium phenoxide) 7, a structurally well-defined reagent that holds two sites of strong Lewis acidity in close proximity. Bidentate Lewis acid 7 forms a crystalline 1:2 complex with 4,4'-dimethylbenzophenone. An x-ray crystallog. study revealed that each atom of Ti binds only one mol. of ketone to form an unusual pentacoordinate adduct with an approx. trigonal bipyramidal geometry. Treatment of fluorenediol 3 with 2 equiv of  $\text{AlEt}_3$  does not yield the expected bis(diethylaluminum phenoxide) but rather its dimer 9. Formation of diverse reagents 7 and 9 from the same precursor demonstrates that the strategy of converting organic compds. with suitably oriented hydroxyl groups into the corresponding metal alkoxides is a particularly versatile and effective way to make strong, structurally well-defined multidentate Lewis acids.

IT 205992-07-0P 205992-09-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 205992-07-0 CAPLUS

CN Titanium, [ $\mu$ -{2,7-bis(1,1-dimethylethyl)-9H-fluorene-1,8-diolato(2-)- $\kappa\text{O}:\kappa\text{O}'$ }]bis[bis(4-methylphenyl)methanone]hexachlorodi-, stereoisomer, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

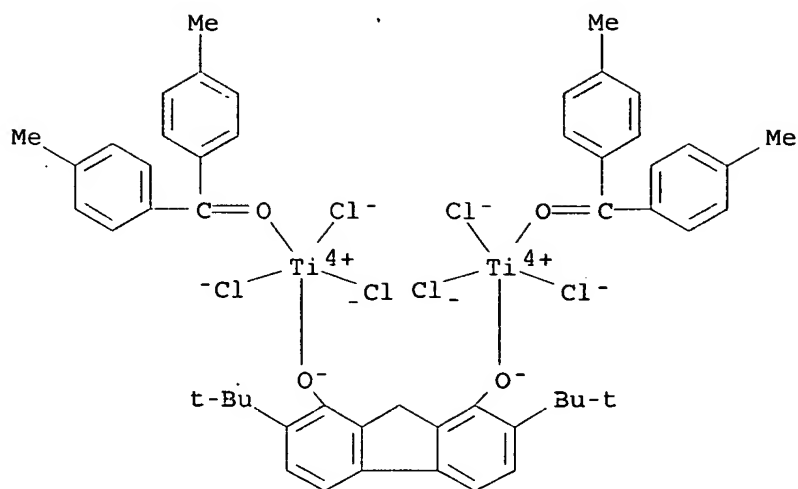
CM 1

CRN 205992-06-9

CMF C51 H52 Cl6 O4 Ti2

CCI CCS



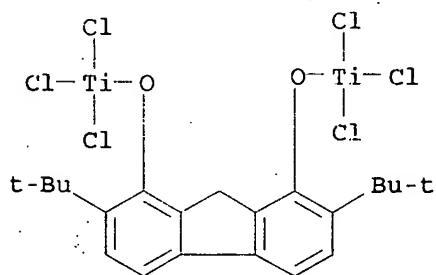


CM 2

CRN 75-09-2  
CMF C H2 Cl2

Cl-CH<sub>2</sub>-Cl

RN 205992-09-2 CAPLUS  
CN Titanium, [ $\mu$ -[2,7-bis(1,1-dimethylethyl)-9H-fluorene-1,8-diolato(2-)-  
κO:κO']]hexachlorodi- (9Cl) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1998:127000 CAPLUS  
DOCUMENT NUMBER: 128:140749  
TITLE: Novel Complexes of Strong Bidentate Lewis Acids  
Derived from 2,2'-(1,3-Butadiyne-1,4-diyl)bis[phenol]  
AUTHOR(S): Saied, Okba; Simard, Michel; Wuest, James D.  
CORPORATE SOURCE: Departement de Chimie, Universite de Montreal,  
Montreal, QC, H3C 3J, Can.  
SOURCE: Organometallics (1998), 17(6), 1128-1133  
CODEN: ORGND7; ISSN: 0276-7333  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Treatment of 2,2'-(1,3-butadiyne-1,4-diyl)bis[6-(1,1-dimethylethyl)-4-methylphenol] (1) with 2 equiv of Al(i-Bu)<sub>3</sub> converts the two hydroxyl

groups into  $\text{OAl}(\text{i-Bu})_2$  groups, thereby transforming diphenol 1 into the corresponding bis(di-i-butylaluminum phenoxide) 8, which holds two strongly Lewis acidic atoms of aluminum in a potentially convergent orientation. Bidentate Lewis acid 8 forms a crystalline 1:1 adduct with 1,2-dimethoxyethane (DME). An x-ray crystallog. study revealed that the adduct is a linear oligomer in which the two Lewis acidic sites of reagent 8 each bind a basic oxygen atom from different mols. of DME. However, low-temperature NMR studies indicated that in solution a discrete 1:1 adduct 9

is

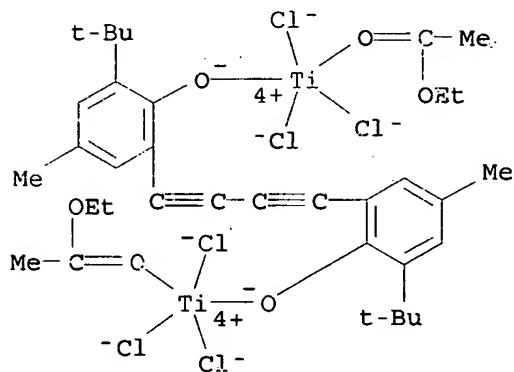
favored, in which the two Lewis acidic sites of reagent 8 each bind one of the two basic sites in a single mol. of DME. Formation of adduct 9 provides an example of the recognition and binding of a multidentate Lewis base by a complementary multidentate Lewis acid. Addition of 2 equiv of  $\text{TiCl}_4$  to diphenol 1 converts the hydroxyl groups into  $\text{OTiCl}_3$  groups and produces the corresponding bis(trichlorotitanium phenoxide) 11, which forms an unusual 1:2 complex with  $\text{CH}_3\text{COOC}_2\text{H}_5$ . An x-ray crystallog. study of this complex established that each Lewis acidic atom of titanium binds only 1 equiv of  $\text{CH}_3\text{COOC}_2\text{H}_5$  to form an unprecedented pentacoordinate adduct with a square-pyramidal geometry. Formation of diverse reagents 8 and 11 from the same precursor demonstrates that the strategy of converting organic compds. with suitably oriented hydroxyl groups into the corresponding metal alkoxides is a versatile and effective way to make multidentate Lewis acids.

IT 202347-65-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 202347-65-7 CAPLUS

CN Titanium,  $[\mu - [[2,2' - (1,3\text{-butadiyne-1,4-diyl})\text{bis}[6 - (1,1\text{-dimethylethyl}) - 4\text{-methylphenolato-}\kappa\text{O}]](2-)]\text{hexachlorobis(ethyl acetate-}\kappa\text{O}')] \text{di-},$   
stereoisomer (9CI) (CA INDEX NAME)

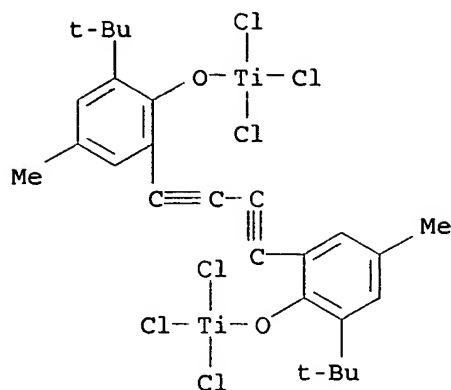


IT 202347-60-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and mol. structure of)

RN 202347-60-2 CAPLUS

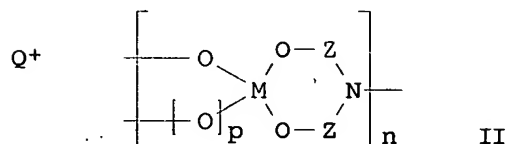
CN Titanium,  $[\mu - [[2,2' - (1,3\text{-butadiyne-1,4-diyl})\text{bis}[6 - (1,1\text{-dimethylethyl}) - 4\text{-methylphenolato-}\kappa\text{O}]](2-)]\text{hexachlorodi-}$  (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD: ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 17 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1997:260113 CAPLUS  
 DOCUMENT NUMBER: 126:308167  
 TITLE: Double alkoxide monomers, oligomers, and polymers  
 INVENTOR(S): Laine, Richard M.; Bickmore, Clint R.; Waldner, Kurt F.  
 PATENT ASSIGNEE(S): Regents of University of Michigan, USA  
 SOURCE: U.S., 19 pp., Cont.-in-part of U.S. 5,418,298.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5614596	A	19970325	US 1995-371911	19950112
US 5419298	A	19950523	US 1993-34531	19930319
US 5958361	A	19990928	US 1995-562296	19951122
PRIORITY APPLN. INFO.:			US 1993-34531	A2 19930319
			US 1995-371911	A2 19950112
OTHER SOURCE(S):	MARPAT 126:308167			
GI				



AB The neutral or mixed ionic-neutral polymetallooxanes have general formula [O'R<sub>3</sub>C(R<sub>1</sub>)(R<sub>2</sub>)O]<sub>n</sub>M' (I) [M<sub>1</sub> = tri- or tetravalent Al or Ga, tetra-, penta-, or hexavalent Si, Ge, Sn, Ti, Zr, or Hf; n = 2, 3 or 4 when M<sub>1</sub> is Al or Ga; n = 3, 4, 5, or 6 when M<sub>1</sub> is Si, Ge, Sn, Ti, Zr, or Hf; independently, R<sub>1</sub>, R<sub>2</sub> is ≥1 of H, OH, C<sub>1</sub>-8-alkyl, C<sub>1</sub>-6-alkoxy, C<sub>2</sub>-8-alkenyl, C<sub>6</sub>-12-aryl, C<sub>1</sub>-8-hydroxyalkyl, C<sub>1</sub>-8-thioalkyl, C<sub>2</sub>-12-alkoxyalkyl, C<sub>4</sub>-20-heteroarom., C<sub>1</sub>-10-alkylsilane, C<sub>1</sub>-10-alkylsiloxane; O' is bonded to M<sub>1</sub>, M<sub>2</sub>, or H (M<sub>2</sub> = Si, Ge, Sn, Al, Ga, Ti, Zr, Hf, an ammonium species, a phosphonium species, Group IA element, IIA element; wherein when one O' is bonded to M<sub>1</sub>, n is 2 or 3 when M<sub>1</sub> is Al, or Ga, and ≥1 O' is bonded to M<sub>2</sub>; when one O' is

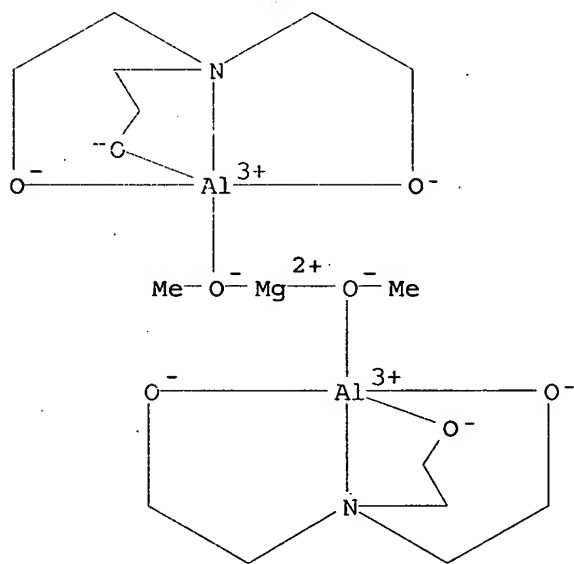
bonded to M1, n is 3, 4, or 5 when M1 is Si, Ge, Sn, Ti, Zr, or Hf, and  $\geq 1$  O' is bonded to M2; and when 2 O' are bonded to M1 and M1 is Si, Ge, Sn, Ti, Zr, or Hf, n is 3 or 4 and  $\geq 1$  O' is bonded to M2); independently, R3 is  $\geq 1$  of (CR2)y, (CR2CR2)y, [(CR2CR2)yO]y(CR2)y (R is  $\geq 1$  of H, OH, C1-8-alkyl, C1-6-alkoxy, C2-8-alkenyl, C6-12-aryl, C1-8-hydroxyalkyl, C1-8-thioalkyl, C2-12-alkoxyalkyl, C4-20-heteroarom., C1-10-alkylsilane, C1-10-alkylsiloxane; y = 1 to 10; and the polymetallooxane contains  $\geq 1$  M2)]. The polymetallooxanes contain the heterocyclic moiety (II) (M = Al, Ga, Si, Ge, Sn, Ti, Zr, Hf; when M = Al or Ga, p = 0 or 1; when M = Si, Ge, Sn, Ti, Zr, or Hf, p = 1, 2, 3; when M = Al or Ga and p = 1, Q+ is Group IA or IIA counterion, ammonium counterion having general formula R4N, or phosphonium counterion having general formula R4P+; when p = 0, Q+ is not present; when M = Si, Ge, Sn, Ti, Zr, or Hf, and p = 2 or 3, Q+ = Group IA or IIA counterion, ammonium counterion having general formula R4N, or phosphonium counterion having general formula R4P+; when p = 1, Q+ is not present; R as above; Z is residue of amine reactant; n = 1-150). The manufacture of the polymetallooxanes employing inexpensive metal sources, e.g., sand, Al2O3, and rutile, comprises dissolving  $\geq 1$  IIIA, IVA, IVB metaloxy compds., e.g., oxides, hydroxides, or hydrates, with a di- or polyhydroxyl compound in the presence of an amine or alkanolamine. The mixed polymetallooxanes and homo-polymetallooxanes obtained are suitable for preparing coatings, fibers, powders, ceramics, and glass.

IT 189184-10-9P

RL: IMF (Industrial manufacture); PREP (Preparation)  
(double alkoxide monomers, oligomers, and polymers, and their manufacture)

RN 189184-10-9 CAPLUS

CN Magnesium, di- $\mu$ -methoxybis[[[2,2',2''-(nitrilo- $\kappa$ N)tris[ethanolato- $\kappa$ O]](3-)]aluminum]- (9CI) (CA INDEX NAME)



L6 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:513360 CAPLUS

DOCUMENT NUMBER: 125:264326

TITLE: Titanium(IV) alkoxides with mono- and bidentate ligands

AUTHOR(S): Mahrwald, Rainer; Ziemer, Burkhard; Ramm, Matthias

CORPORATE SOURCE: Fachbereich Chem., Humboldt-Univ., Berlin, D-10115, Germany

SOURCE: Journal fuer Praktische Chemie/Chemiker-Zeitung

(1996), 338(6), 583-585  
CODEN: JPCCEM; ISSN: 0941-1216

PUBLISHER: Barth  
DOCUMENT TYPE: Journal  
LANGUAGE: English

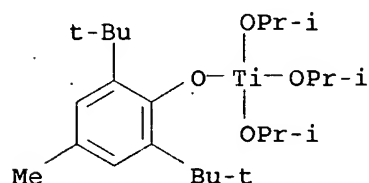
AB Ti(IV) alkoxides containing mono- and bidentate ligands were prepared in good yields by transesterification of Ti(OiPr)<sub>4</sub>. The crystal structures of (Ph<sub>3</sub>CO)<sub>3</sub>TiOiPr and (iPrO)<sub>2</sub>Ti[O(CPh<sub>2</sub>)<sub>2</sub>O] are reported.

IT 151041-46-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 151041-46-2 CAPLUS

CN Titanium, [2,6-bis(1,1-dimethylethyl)-4-methylphenolato]tris(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:243654 CAPLUS

DOCUMENT NUMBER: 122:62062

TITLE: Synthesis and characterization of Group IV metal  
adamantanol alkoxides as potential PZT  
precursors

AUTHOR(S): Boyle, Timothy J.; Pearson, Aaron T.; Schwartz, Robert  
W.

CORPORATE SOURCE: Advanced Materials Laboratory, Sandia National  
Laboratories, Albuquerque, NM, 87106, USA

SOURCE: Ceramic Transactions (1994), 43 (Ferroic Materials:  
Design, Preparation, and Characteristics), 79-87  
CODEN: CETREW; ISSN: 1042-1122

DOCUMENT TYPE: Journal

LANGUAGE: English

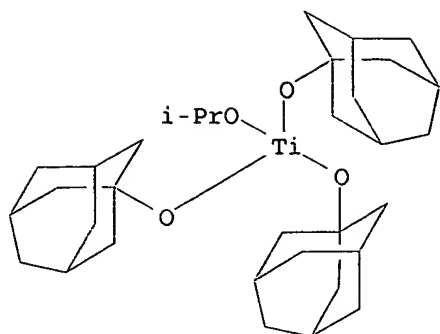
AB The size and morphol. of adamantanol (AdamO-H) make it an interesting ligand to investigate as a possible starting reagent for the generation of lead zirconate titanate (PZT) thin films. It was believed that hydrolysis, due to ambient humidity, would be reduced as the steric bulk around the metal center was increased. Group IV (Ti, Zr) metal alkoxides were reacted, in sundry stoichiometries, with adamantanol and the resulting compds. were used for film generation. Surprisingly, most of these compds. crystallized when their solns. were spin-cast deposited onto silicon substrates. The one exception was the (AdamO)Zr(OCHMe<sub>2</sub>)<sub>3</sub> compound, which apparently gelled. Ellipsometric data obtained on this film showed that typical densification occurred.

IT 160262-98-6P 160262-99-7P 160263-00-3P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(precursors; preparation and characterization of adamantanol  
alkoxides as potential PZT precursors)

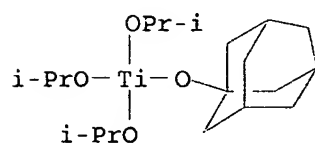
RN 160262-98-6 CAPLUS

CN Titanium, (2-propanolato)tris(tricyclo[3.3.1.1<sup>3,7</sup>]decan-1-olato)-, (T-4)- (9CI) (CA INDEX NAME)



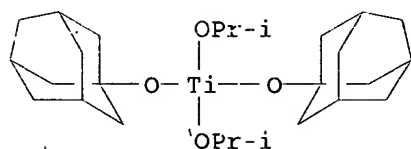
RN 160262-99-7 CAPLUS

CN Titanium, tris(2-propanolato)(tricyclo[3.3.1.1.3,7]decan-1-olato)-, (T-4)-(9CI) (CA INDEX NAME)



RN 160263-00-3 CAPLUS

CN Titanium, bis(2-propanolato)bis(tricyclo[3.3.1.1.3,7]decan-1-olato)-, (T-4)-(9CI) (CA INDEX NAME)



L6 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:644187 CAPLUS

DOCUMENT NUMBER: 121:244187

TITLE: Preparation of Titanium Fluoroalkoxides by Alcoholysis of Titanium **Alkoxides**

AUTHOR(S): Campbell, Carolyn; Bott, Simon G.; Larsen, Raymond; Van Der Sluys, William G.

CORPORATE SOURCE: Department of Chemistry, University of Montana, Missoula, MT, 59812, USA

SOURCE: Inorganic Chemistry (1994), 33(22), 4950-8

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction of  $Ti(OR)_4$  where R = isoPr and Et with >4 equiv of fluoroalcs., HORf [Rf =  $CH(CF_3)_2$ ,  $C_6F_5$ , 2,6-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 2,4-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 4-FC<sub>6</sub>H<sub>4</sub>, Ph], gave a series of  $Ti(ORf)_x(OR)_{4-x}(HOR)_n$  compds. where x = 2-4 and n = 0 or 1. Only in the cases of Rf =  $CH(CF_3)_2$  (x = 2) and 2,6-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub> (x = 2 and 3) does n = 0. The degree of substitution can be correlated to the electron-withdrawing ability of the Rf group, with highly electron-withdrawing groups do not favor complete substitution. These compds. were characterized by combustion elemental anal. and IR and <sup>1</sup>H and <sup>19</sup>F NMR spectroscopies. Single-crystal x-ray diffraction studies of  $Ti(ORf)_x(OR)_{4-x}(HOR)_n$  [Rf =  $CH(CF_3)_2$ , R = Et, and x = 2; Rf =  $C_6F_5$ , R = isoPr, and x = 3], revealed centrosym. dinuclear structures held together by bridging O atoms. The coordination geometries approx. edge-shared

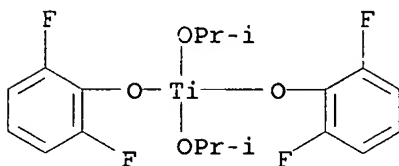
bioctahedra with the coordinated alcs. H-bonding across the dinuclear unit to an O atom of an alkoxide. Crystal data for  $[\text{Ti}\{\text{OCH}(\text{CF}_3)_2\}_2(\text{OEt})_2(\text{HOEt})]_2$  at 25°: a 10.233(3), b 12.702(4), c 16.175(7) Å,  $\beta$  96.05(3)°, Z = 2, dc = 1.646 g cm<sup>-3</sup>, space group P21/n, R = 0.074, and Rw = 0.076. Crystal data for  $[\text{Ti}(\text{OC}_6\text{F}_5)_3(\text{OCHMe}_2)(\text{HOCHMe}_2)]_2 \cdot \text{C}_7\text{H}_8$  at 25°: a 11.1009(9), b 19.388(1), c 14.397(1) Å,  $\beta$  92.805(6)°, Z = 2, dc = 1.636 g cm<sup>-3</sup>, space group P21/n, R = 0.0773, and Rw = 0.0879. The x-ray crystal structure of  $[\text{Ti}(\text{O}-2,6\text{-F}_2\text{C}_6\text{H}_3)_3(\text{OCHMe}_2)]_2$  also was determined. The coordination geometry defined by the O atoms of the alkoxide ligands approximates a square-based pyramid, with an isopropoxide in the apical site [Ti(1)-O(4) = 1.718(6) Å and Ti(1)-O(4)-C(4) = 159.6(6)°]. One of the terminal phenoxides has a nearly linear angle [169.3(6)°], while the other has a relatively acute angle [123.3(4)°]. The Ph group of the latter is oriented such that a F fills the site trans to the isopropoxide. Ti(1)-F(1) = 2.704(5) Å is virtually identical to the sum of the van der Waals radii of F and Ti(IV). Crystal data at 25°: a 11.4404(9), b 18.927(2), c = 10.830(1) Å,  $\beta$  114.968(7)°, Z = 2, dc = 1.541 g cm<sup>-3</sup>, space group P21/c, R = 0.0564 and Rw = 0.0573. The two compds. that do not coordinate alc. [R = Me<sub>2</sub>CH; Rf = 2,6-F<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, x = 3, and Rf = CH(CF<sub>3</sub>)<sub>2</sub>, x = 2], also do not form stable complexes with Lewis bases such as MeCN or THF. This contrasts with Ti[OCH(CF<sub>3</sub>)<sub>2</sub>]<sub>4</sub>, which forms volatile Ti[OCH(CF<sub>3</sub>)<sub>2</sub>]<sub>4</sub>L<sub>2</sub> [L = MeC.tplbond.N and THF] compds. The structure of Ti[OCH(CF<sub>3</sub>)<sub>2</sub>]<sub>4</sub>(N.tplbond.CMe)<sub>2</sub> was determined using x-ray crystallog. The nitrile ligands occupy cis positions in the distorted octahedral coordination geometry. Crystal data for at 25°: a 10.2872(7), b 15.295(1), c 18.651(1) Å, Z = 4, dc = 1.811 g cm<sup>-3</sup>, space group C2221, R = 0.0583, and Rw = 0.0550.

IT 158472-28-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 158472-28-7 CAPLUS

CN Titanium, bis(2,6-difluorophenolato)bis(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:557203 CAPLUS

DOCUMENT NUMBER: 121:157203

TITLE: Preparation of linear oligoaniline derivatives using titanium alkoxide as a condensing agent

AUTHOR(S): Ochi, Miyoko; Furusho, Hitoshi; Tanaka, Jun

CORPORATE SOURCE: Fac. Eng., Sci. Univ. Tokyo, Tokyo, 162, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1994), 67(6), 1749-52

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:157203

AB Linear oligoaniline derivs. were prepared by the reaction of aromatic amines and phenols using various titanium alkoxides as condensing agents. The oligomers obtained were silver white microscopic crystals. Titanium alkoxides used were titanium alkoxide or titanium alkoxide aryloxy and the latter showed high

dehydration condensation activity in comparison with the usual titanium alkoxides.

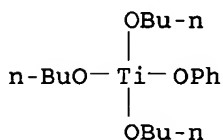
IT 157446-67-8 157446-68-9 157446-69-0  
157475-56-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation as catalyst for preparation of linear oligoaniline derivs.)

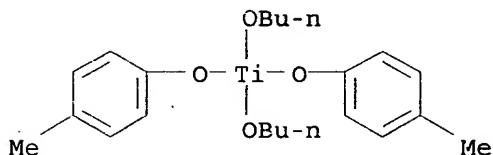
RN 157446-67-8 CAPLUS

CN Titanium, tributoxyphenoxy-, (T-4)- (9CI) (CA INDEX NAME)



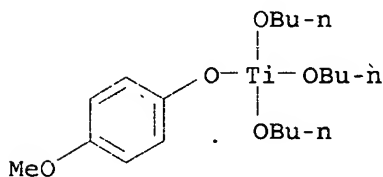
RN 157446-68-9 CAPLUS

CN Titanium, dibutoxybis(4-methylphenolato)-, (T-4)- (9CI) (CA INDEX NAME)



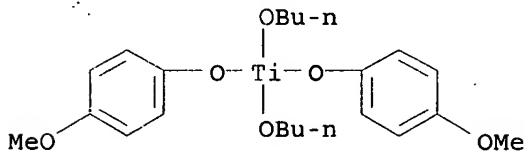
RN 157446-69-0 CAPLUS

CN Titanium, tributoxy(4-methoxyphenolato-O1)-, (T-4)- (9CI) (CA INDEX NAME)



RN 157475-56-4 CAPLUS

CN Titanium, dibutoxybis(4-methoxyphenolato-O1)-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:9792 CAPLUS

DOCUMENT NUMBER: 120:9792

TITLE: Crystalline polymer compositions with improved transparency and mechanical strength

INVENTOR(S): Kimura, Ryoji; Tsuboi, Tetsuo; Nishikawa, Kazunori

PATENT ASSIGNEE(S): Asahi Denka Kogyo KK, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

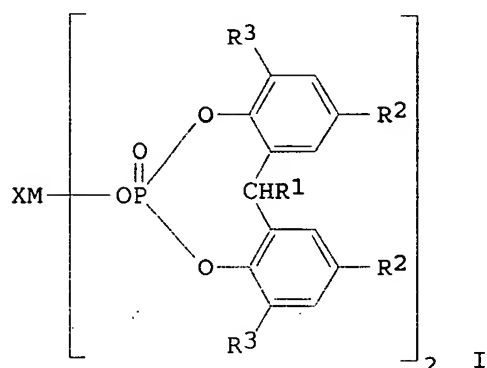
DOCUMENT TYPE: Patent



LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05156078	A2	19930622	JP 1991-322153	19911205
JP 3046428	B2	20000529		
US 5342868	A	19940830	US 1993-26479	19930304
EP 622404	A1	19941102	EP 1993-105144	19930329
EP 622404	B1	19980708		
R: BE, CH, DE, ES, FR, GB, LI, LU, NL				
ES 2118847	T3	19981001	ES 1993-105144	19930329
PRIORITY APPLN. INFO.:			JP 1991-302056	A 19911118
			JP 1991-322153	A 19911205
			EP 1993-105144	A 19930329

GI



AB The title compns. contain (A) 100 parts crystalline synthetic polymers, (B) 0.01-5 parts alkali metal salts of carboxylic acids,  $\beta$ -diketones, and/or  $\beta$ -ketoacetate esters, and (C) 0.015-5 parts multivalent metal salts of cyclic organic phosphate esters I [R1 = H, C1-4 alkyl; R2, R3 = H, C1-12 alkyl; M = Group III or IV metals; X = OH when M = Group III metals, O or (HO)2 when M = Group IV metals]. Thus, 3:97 ethylene-propylene copolymer (melt flow rate 5.0 g/10-min) 100, tetrakis[methylene-3-(3,5-di-tert-butylphenyl)propionato]methane 0.1, tris(2,4-di-tert-butylphenyl) phosphite 0.1, I (R1 = H, R2 = R3 = Me3C; M = Al, X = OH) 0.1, and Li laurate 0.1 part were melt kneaded, pelletized, and injection molded to give a test piece showing Haze 5% initially and 7% after 36 h in H2O at 80°.

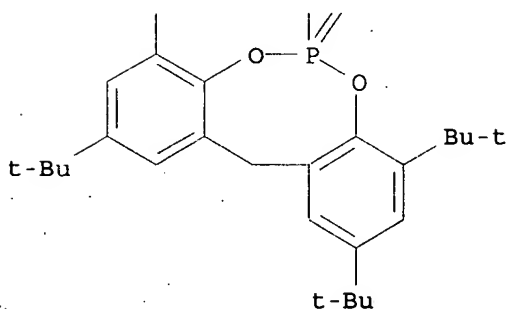
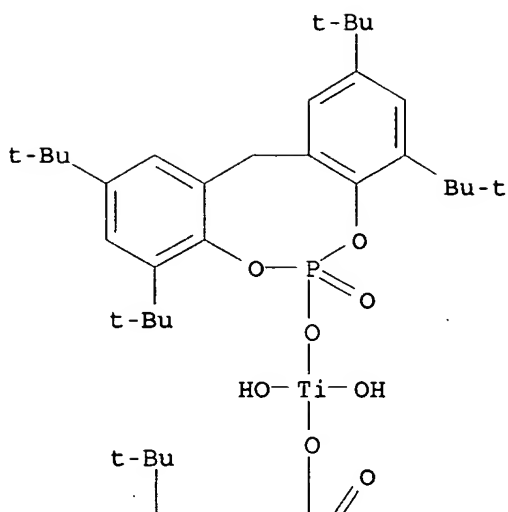
IT 151810-82-1

RL: USES (Uses)

(nucleating agents, crystalline polypropylene compns. containing, with alkali metal salts, for improved transparency and impact strength)

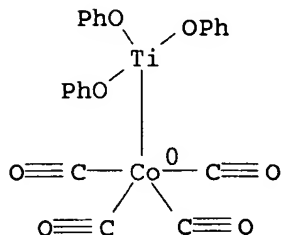
RN 151810-82-1 CAPLUS

CN Titanium, dihydroxybis[2,4,8,10-tetrakis(1,1-dimethylethyl)-6-(hydroxy- $\kappa$ O)-12H-dibenzo[d,g][1,3,2]dioxaphosphocin 6-oxidato]-, (T-4)- (9CI)  
 (CA INDEX NAME)

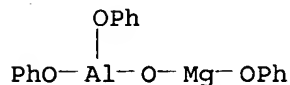


L6 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:594301 CAPLUS  
 DOCUMENT NUMBER: 119:194301  
 TITLE: Heterodinuclear titanium-cobalt complexes: syntheses and properties. X-ray structure of [(tert-C<sub>4</sub>H<sub>9</sub>O)<sub>3</sub>TiCo(CO)<sub>4</sub>](Ti-Co)  
 AUTHOR(S): Selent, Detlef; Bäckhaus, Ruediger; Pickardt, Joachim  
 CORPORATE SOURCE: Zent. Heterog. Katal., Berlin, O-1199, Germany  
 SOURCE: Organometallics (1993), 12(7), 2857-60  
 CODEN: ORGND7; ISSN: 0276-7333  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB An x-ray structural study establishes an unbridged Ti-Co bond in [(Me<sub>3</sub>CO)<sub>3</sub>TiCo(CO)<sub>4</sub>] (I) and shows it crystallizes as orthorhombic, space group Pbn21, a 1192.5(7), b 1375.8(9), c 1405.0(10) pm, Z = 4. The variation of the alkoxide ligand leads to the more thermally unstable derivs. [(RO)<sub>3</sub>TiCo(CO)<sub>4</sub>] (R = CHMe<sub>2</sub>, CH(CF<sub>3</sub>)<sub>2</sub>, Ph), whereas trans-[(Me<sub>3</sub>CO)<sub>3</sub>TiCo(CO)<sub>3</sub>(PPh<sub>3</sub>)] is formed in a selective axial CO ligand substitution reaction between I and PPh<sub>3</sub>.

IT 150429-80-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 150429-80-4 CAPLUS  
 CN Titanium, triphenoxy(tetracarbonylcobalt)-, (Co-Ti), stereoisomer (9CI)  
 (CA INDEX NAME)



L6 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1993:168766 CAPLUS  
 DOCUMENT NUMBER: 118:168766  
 TITLE: Specific catalytic properties of monomeric and  
 oligomeric metal phenoxides  
 AUTHOR(S): Perchenko, V. N.; Abubakirov, R. Sh.; Kurashev, M. V.;  
 Semenov, O. B.; Khrapova, I. M.; Plate, N. A.  
 CORPORATE SOURCE: Inst. Neftekhim. Sint., Moscow, Russia  
 SOURCE: Doklady Akademii Nauk (1992), 326(2), 276-8 [Chem.]  
 CODEN: DAKNEQ; ISSN: 0869-5652  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Alkylation of phenol by styrene catalyzed by R(OPh)<sub>3</sub> (R = Al, B), R(OPh)<sub>2</sub>  
 (R = Mg, Ca), (PhO)<sub>2</sub>AlOAl(OPh)<sub>2</sub>, (PhO)<sub>2</sub>AlOMgOPh, and  
 [(PhO)<sub>2</sub>Al(OAlOPh)<sub>n</sub>OAl(OPh)<sub>2</sub> n = 5-28], gave, depending on the catalyst,  
 3-99% alkylphenol and 1-98% oligoalkylphenol. Thus, alkylation catalyzed  
 by Al(OPh)<sub>3</sub> at 140° gave 97-99% o-PhCHMeC<sub>6</sub>H<sub>4</sub>OH (I) and 1-3%  
 oligoalkylphenol; alkylation catalyzed by Ca(OPh)<sub>3</sub> gave 97-98%  
 oligoalkylphenol (mol. weight 76000-78200) and 2-3% I.  
 IT 146307-35-9  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalyst, for alkylation of phenol by styrene)  
 RN 146307-35-9 CAPLUS  
 CN Magnesium, (diphenoxyaluminum)-μ-oxophenoxy- (9CI) (CA INDEX NAME)



L6 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1992:650846 CAPLUS  
 DOCUMENT NUMBER: 117:250846  
 TITLE: Spectroscopic studies on the TiCl<sub>4</sub>-promoted reaction  
 of allylsilanes with aldehydes and  
 α,β-enones  
 AUTHOR(S): Denmark, Scott E.; Almstead, Neil G.  
 CORPORATE SOURCE: Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA  
 SOURCE: Tetrahedron (1992), 48(27), 5565-78  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:250846

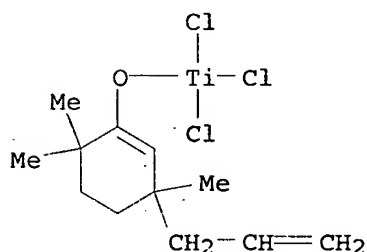
AB Spectral examination of the complexation of n-heptanal or 4-(n-heptyl)benzaldehyde with  $\text{TiCl}_4$  showed that the nature of the complex formed was dependent upon the stoichiometry of  $\text{TiCl}_4$  present. The 2:1 (Lewis base/ $\text{TiCl}_4$ ) complex was preferred at substoichiometric quantities of  $\text{TiCl}_4$ ; the 1:1 complex formed preferentially when excess  $\text{TiCl}_4$  was present. Reaction of the precomplexed aldehyde with allyltrimethylsilane (I) led to the formation of a titanium alkoxide, the structure of which was independently established by metathesis of the corresponding silyl ether. No metathesis of I occurred before addition. The reaction of I with  $\text{TiCl}_4$ -complexed enones was also examined. A Ti enolate was observed spectrally as the intermediate in this reaction. No metathesis of I occurred before addition to the complexed enone.

IT 144527-99-1 144528-03-0

RL: PRP (Properties)  
(carbon-13 NMR of)

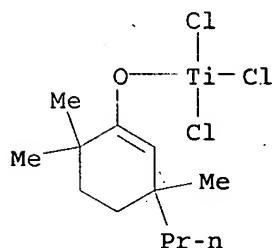
RN 144527-99-1 CAPLUS

CN Titanium, trichloro[3,6,6-trimethyl-3-(2-propenyl)-1-cyclohexen-1-olato]-, (T-4)- (9CI) (CA INDEX NAME)



RN 144528-03-0 CAPLUS

CN Titanium, trichloro(3,6,6-trimethyl-3-propyl-1-cyclohexen-1-olato)-, (T-4)- (9CI) (CA INDEX NAME)



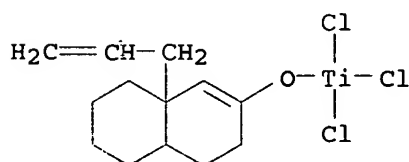
IT 144527-96-8P 144527-97-9P 144527-98-0P

144527-99-1P

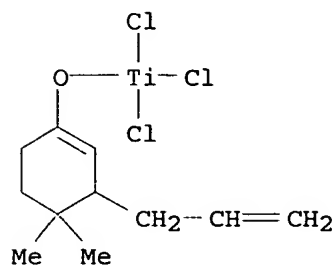
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and carbon-13 NMR of)

RN 144527-96-8 CAPLUS

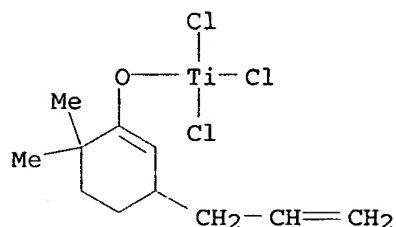
CN Titanium, trichloro[3,4,4a,5,6,7,8,8a-octahydro-8a-(2-propenyl)-2-naphthalenolato]-, (T-4)- (9CI) (CA INDEX NAME)



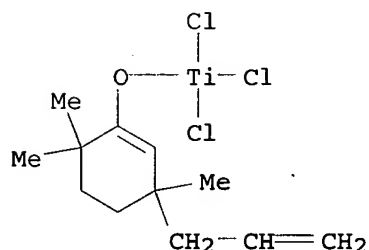
RN 144527-97-9 CAPLUS  
 CN Titanium, trichloro[4,4-dimethyl-3-(2-propenyl)-1-cyclohexen-1-olato]-,  
 (T-4)- (9CI) (CA INDEX NAME)



RN 144527-98-0 CAPLUS  
 CN Titanium, trichloro[6,6-dimethyl-3-(2-propenyl)-1-cyclohexen-1-olato]-,  
 (T-4)- (9CI) (CA INDEX NAME)



RN 144527-99-1 CAPLUS  
 CN Titanium, trichloro[3,6,6-trimethyl-3-(2-propenyl)-1-cyclohexen-1-olato]-,  
 (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:194374 CAPLUS

DOCUMENT NUMBER: 116:194374

TITLE: Cyclopentadienylmagnesium alkoxides derived from polyfunctional alcohols

AUTHOR(S): Nicola, O.; Mackey, D.; Morley, Christopher P.

CORPORATE SOURCE: Dep. Chem., Queen's Univ. Belfast, Belfast, BT9 5AG, UK

SOURCE: Journal of Organometallic Chemistry (1992), 426(3), 279-85

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:194374

AB Magnesocene (1) reacts with polyfunctional alcs. (2a, N,N-dimethylethanolamine; 2b, 2-ethoxyethanol; 2c, 2-(2-ethoxyethoxy)ethanol;

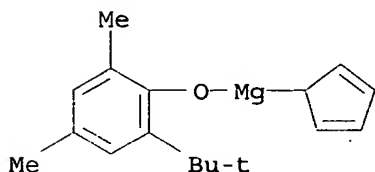
2d, 2-[[[(2-dimethylamino)ethyl)methylamino]ethanol] to yield polymeric cyclopentadienylmagnesium alkoxides  $[(\eta\text{-C}_5\text{H}_5)\text{MgOR}]_x$  (3a-d). Compds. 3a-d dissolve in pyridine to yield solns. containing pyridine adducts of the corresponding monomers. These compds. all appear to contain formally 12-electron, pseudo-6-coordinate magnesium. Compound 1 reacts with 2,4-dimethyl-6-tert-butylphenol to form cyclopentadienyl (2,4-dimethyl-6-tert-butylphenoxy)magnesium, in which the steric bulk of the phenoxide ligand stabilizes the monomeric, 8-electron configuration.

IT 140848-04-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 140848-04-0 CAPLUS

CN Magnesium, 2,4-cyclopentadien-1-yl[2-(1,1-dimethylethyl)-4,6-dimethylphenolato]- (9CI) (CA INDEX NAME)



L6 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:156006 CAPLUS

DOCUMENT NUMBER: 114:156006

TITLE: Toward supported catalyst models: the synthesis, characterization, redox chemistry, and structures of titanium tetrakis(aryloxy) complexes [aryl =  $\text{C}_6\text{H}_4(2\text{-tert-Bu})$ ,  $\text{C}_6\text{H}_4(2,3,5,6\text{-Me}_4)$ ]

AUTHOR(S): Toth, Robert T.; Stephan, Douglas W.

CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Windsor, Windsor, ON, N9B 3P4, Can.

SOURCE: Canadian Journal of Chemistry (1991), 69(1), 172-8  
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction of substituted phenoxides with  $\text{TiCl}_4$  affords  $\text{Ti}(\text{OC}_6\text{H}_4\text{Me}_3\text{-}2)_4$  (I) and  $\text{Ti}(\text{OC}_6\text{HMe}_4\text{-}2,3,5,6)_4$  (II). I crystallizes as tetragonal, space group  $P4_2/c$ ,  $a$  15.203(4),  $c$  8.026(3) Å,  $Z = 2$ ,  $R = 0.053$ ,  $R_w = 0.065$ . II crystallizes as orthorhombic, space group  $Pbcn$ ,  $a$  16.539(7),  $b$  16.136(6),  $c$  27.716(12) Å,  $Z = 8$ ,  $R = 0.087$ ,  $R_w = 0.082$ . The geometry of the Ti coordination sphere in these complexes is best described as pseudo-tetrahedral. For I strict crystallographic 4-fold symmetry is imposed. II exhibits reversible cyclic voltammetric behavior consistent with a 1 electron reduction to the Ti(III) analog. Chemical reduction of II using

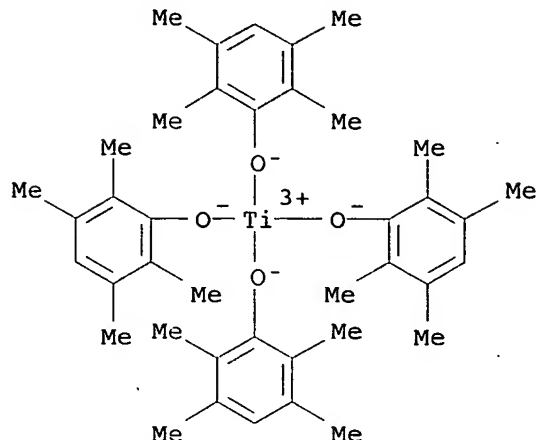
NaH affords the quant. formation of  $(2,3,5,6\text{-Me}_4\text{C}_6\text{HO})_2\text{Ti}(\mu\text{-OC}_6\text{HMe}_4\text{-}2,3,5,6)_2\text{Na}(\text{THF})_2$  (III). The reaction of III with  $[(\text{COD})\text{Rh}(\mu\text{-Cl})]_2$  (COD = 1,5-cyclooctadiene) does not afford the Ti(III)/Rh(I) early-late heterobimetallic (ELHB) complex  $(2,3,5,6\text{-Me}_4\text{C}_6\text{HO})_2\text{Ti}(\mu\text{-OC}_6\text{HMe}_4\text{-}2,3,5,6)_2\text{Rh}(\text{COD})$ . The nature of all products is not known; redox chemical, in which electron transfer from Ti(III) to Rh(I) occurs is evidenced by the generation of II and Rh(0). Ligand transfer reactions giving uncharacterized Rh-alkoxide are suggested by the spectral data. The implications and ramifications for the synthesis of alkoxide bridged ELHB models of bimetallic heterogeneous catalyst systems are discussed.

IT 132805-11-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(ESR and elec. potential of couple containing)

RN 132805-11-9 CAPLUS

CN Titanate(1-), tetrakis(2,3,5,6-tetramethylphenolato)-, (T-4)- (9CI) (CA INDEX NAME)



IT 132805-12-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and ESR and reaction of, with rhodium chloro cyclooctadiene dinuclear complex)

RN 132805-12-0 CAPLUS

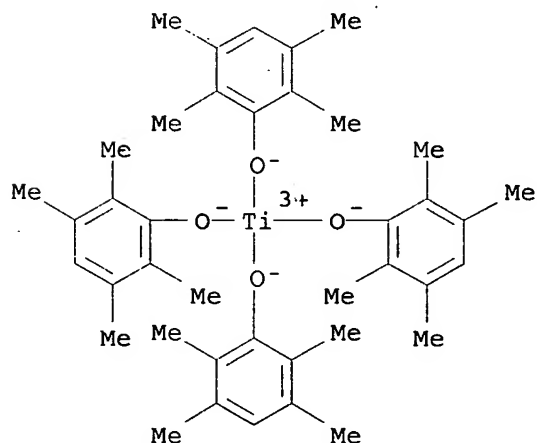
CN Sodium(1+), bis(tetrahydrofuran)-, (T-4)-tetrakis(2,3,5,6-tetramethylphenolato)titanate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 132805-11-9

CMF C40 H52 O4 Ti

CCI CCS

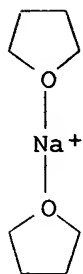


CM 2

CRN 45955-61-1

CMF C8 H16 Na O2

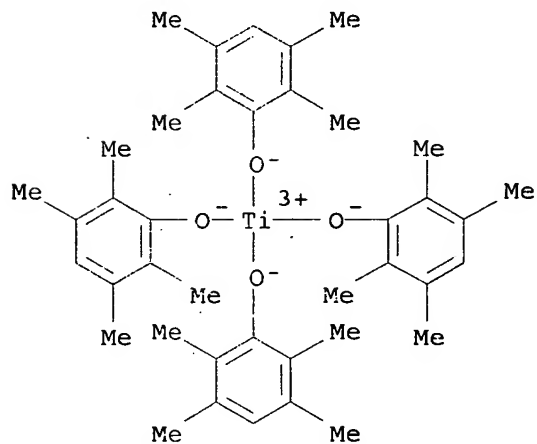
CCI CCS



IT 132805-12-0DP, reaction products with rhodium chloro  
cyclooctadiene dimer  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 132805-12-0 CAPLUS  
CN Sodium(1+), bis(tetrahydrofuran)-, (T-4)-tetrakis(2,3,5,6-  
tetramethylphenolato)titanate(1-) (9CI) (CA INDEX NAME)

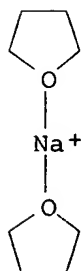
CM 1

CRN 132805-11-9  
CMF C40 H52 O4 Ti  
CCI CCS



CM 2

CRN 45955-61-1  
CMF C8 H16 Na O2  
CCI CCS





ACCESSION NUMBER: 1990:514471 CAPLUS

DOCUMENT NUMBER: 113:114471

TITLE: Stereochemical evidence for a single-electron-transfer (SET) mechanism. Part 2. Reduction of cyclic ketones by alkoxymetal halides

AUTHOR(S): Nasipuri, Dhanonjoy; Saha, Arabinda

CORPORATE SOURCE: Indian Inst. Chem. Biol., Calcutta, 700 032, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1990), 29B(5), 471-3

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

AB New evidence supporting a single-electron-transfer (SET) mechanism in the reduction of cyclic ketones with R<sub>2</sub>CHOM (M = AlCl<sub>2</sub>, Li, MgBr) included the formation of an overwhelming excess of equatorial alcs. from cyclohexanones under conditions in which the metal alkoxides generate strongly paramagnetic solns., identical product composition when 4-tert-butylcyclohexanone is reduced with reagents derived from an exo-endo pair of bicyclic alcs., the isotope effect, and the solvent effect. An explanation in terms of orbital interaction is given to rationalize the almost exclusive formation of equatorial alcs. through the SET mechanism.

IT 94599-62-9 129118-65-6 129118-68-9  
129118-70-3

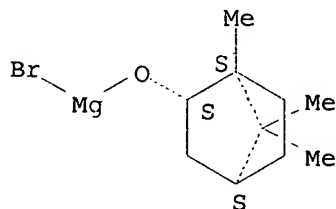
RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction by, of tert-butylcyclohexanone, mechanism and stereochem. of).

RN 94599-62-9 CAPLUS

CN Magnesium, bromo(1,7,7-trimethylbicyclo[2.2.1]heptan-2-olato)-, exo- (9CI)  
(CA INDEX NAME)

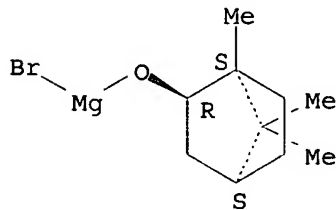
Relative stereochemistry.



RN 129118-65-6 CAPLUS

CN Magnesium, bromo(1,7,7-trimethylbicyclo[2.2.1]heptan-2-olato)-, endo- (9CI) (CA INDEX NAME)

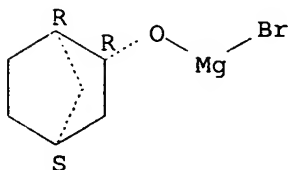
Relative stereochemistry.



RN 129118-68-9 CAPLUS

CN Magnesium, (bicyclo[2.2.1]heptan-2-olato)bromo-, exo- (9CI) (CA INDEX NAME)

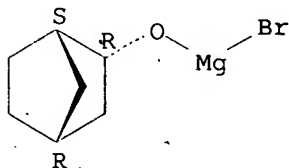
Relative stereochemistry.



RN 129118-70-3 CAPLUS

CN Magnesium, (bicyclo[2.2.1]heptan-2-olato)bromo-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:235510 CAPLUS

DOCUMENT NUMBER: 112:235510.

TITLE: Preparation and characterization of two high oxidation state molybdenum dinitrogen complexes:

[MoCp\*Me3]2(μ-N2) and [MoCp\*Me3](μ-N2)[WCp'Me3]

AUTHOR(S): Schrock, Richard R.; Kolodziej, Richard M.; Liu, Andrew H.; Davis, William M.; Vale, Michael G.

CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (1990), 112(11), 4338-45

CODEN: JACSAT; ISSN: 0002-7963

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:235510

AB [MoCp\*Cl4]2 (Cp\* = η<sup>5</sup>-pentamethylcyclopentadienyl) is alkylated by MeMgCl in THF to give 70% red microcryst. MoCp\*Me4 which reacts with 1 equivalent of HOSO<sub>2</sub>CF<sub>3</sub> in ether to give 85% purple microcryst. MoCp\*Me3(OSO<sub>2</sub>CF<sub>3</sub>) (I). Substitution reaction of I with LiOR (OR = pentafluorophenoxide, 2,6-diisopropylphenoxide, 2,6-dimethoxyphenoxide, 2,4,6-trimethoxyphenoxide, 2,6-dimethyl-4-methoxyphenoxide, catecholate) in ether gave 50-80% MoCp\*Me3(OR) (MoCp\*Me2(cat) in the case of catecholate). Cyclic voltammograms of the MoCp\*Me3(OR) complexes display quasi-reversible oxidation waves in the region 0.29 to -0.50 V, and the complexes were chemically oxidized (with the exception of OR = pentafluorophenoxide and catecholate) with [FeCp<sub>2</sub>][PF<sub>6</sub>] in CH<sub>2</sub>Cl<sub>2</sub> to give complexes of the type [MoCp\*Me3(OR)][PF<sub>6</sub>] as orange-brown microcrystalline powders in 80-90% yield. Addition of 3 equiv of hydrazine to [MoCp\*Me3(OR)][PF<sub>6</sub>] in ether provides [MoCp\*Me3]2(μ-N<sub>2</sub>) (II) in low yield after purification by filtration through alumina and recrystn. from ether. [MoCp\*Me3](μ-N<sub>2</sub>)[WCp'Me3] (III) was prepared by treating WCp'Me3(NNH<sub>2</sub>) (Cp' = η<sup>5</sup>-ethyltetramethylcyclopentadienyl) with [MoCp\*Me3(OR)][PF<sub>6</sub>] in ether in the presence of NEt<sub>3</sub> and is isolated by recrystn. from ether/pentane; it is contaminated with [WCp'Me3]2(μ-N<sub>2</sub>). Addition of excess acid to III in the presence of excess zinc amalgam converts 90% of the coordinated dinitrogen ligand into ammonia (1.80 equiv), whereas II and [WCp'Me3]2(μ-N<sub>2</sub>) under similar conditions yield

less than half of the available nitrogen as ammonia. The crystal structures of II and III are reported.

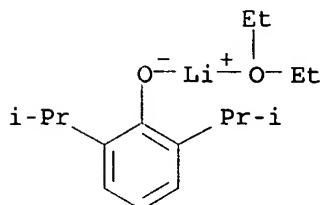
IT 98193-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reaction by, of trimethyl(pentamethylcyclopentadienyl)molybdenum triflate complex)

RN 98193-96-5 CAPLUS

CN Lithium, [2,6-bis(1-methylethyl)phenolato] [1,1'-oxybis[ethane]]- (9CI)  
(CA INDEX NAME)



L6 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:153756 CAPLUS

DOCUMENT NUMBER: 110:153756

TITLE: Conjugate additions of Grignard reagents to  $\alpha,\beta$ -unsaturated ketones mediated by diamine zinc(II) monoalkoxides

AUTHOR(S): Jansen, Johan F. G. A.; Feringa, Ben L.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.

SOURCE: Tetrahedron Letters (1988), 29(29), 3593-6

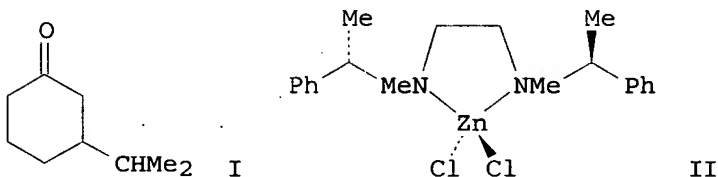
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:153756

GI



AB A method for zinc-mediated 1,4-addns. of Grignard reagents with alkoxides as non-transferable ligands is described. Thus,  $\text{Me}_2\text{CHMgBr}$  was treated with  $\text{Me}_2\text{NCH}_2\text{CH}_2\text{NMe}_2 \cdot \text{ZnCl}_2$  and  $\text{Me}_3\text{COK}$  in THF and then 2-cyclohexenone to give 94% 3-isopropylcyclohexanone (I). Using the chiral zinc complex II  $\leq 14\%$  enantiomeric excess was achieved.

IT 119867-60-6

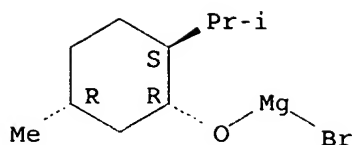
RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. conjugate addition of isopropylmagnesium bromide with cyclohexenone in presence of diamine zinc complex and)

RN 119867-60-6 CAPLUS

CN Magnesium, bromo[5-methyl-2-(1-methylethyl)cyclohexanolato]-, [1R-(1 $\alpha$ ,2 $\beta$ ,5 $\alpha$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:75720 CAPLUS

DOCUMENT NUMBER: 110:75720

TITLE: Chemistry of ( $\eta$ -phenoxide)Cr(CO)<sub>3</sub> ligands

AUTHOR(S): Heppert, Joseph A.; Boyle, Timothy J.; Takusagawa, Fusao

CORPORATE SOURCE: Dep. Chem., Univ. Kansas, Lawrence, KS, 66045, USA

SOURCE: Organometallics (1989), 8(2), 461-7

CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:75720

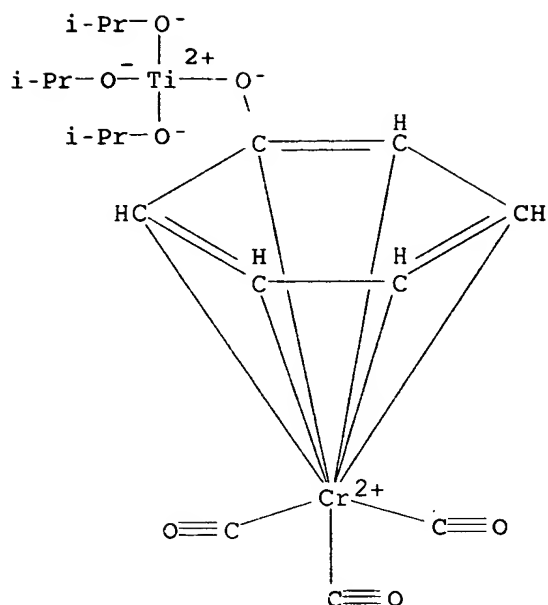
AB (Phenol)tricarbonylchromium complexes are conveniently converted to [ $\eta$ 6-phenoxide)Cr(CO)<sub>3</sub>]- species on treatment with aqueous base. The phenoxide chromium anions, which are readily isolated as crystalline Et<sub>4</sub>N<sup>+</sup> salts, react with main-group electrophiles [(p-tolyl)SO<sub>2</sub>Cl, CF<sub>3</sub>COCl] to produce new sulfonate- and carbonate-substituted arenechromium complexes. Similar reactions between the phenoxide anions and metal electrophiles [CpFe(CO)<sub>3</sub><sup>+</sup> (Cp = cyclopentadienyl), Cp<sub>2</sub>ZrCl<sub>2</sub>] result in electron-transfer reactions that consume the starting arene complexes. Transition metal complexes bearing ( $\eta$ -phenoxide)Cr(CO)<sub>3</sub> ligands are prepared via alcoholysis with metal alkoxide and metal diethylamide precursors. An x-ray crystallog. study of Cp<sub>2</sub>Zr[( $\eta$ -OC<sub>6</sub>H<sub>5</sub>)Cr(CO)<sub>3</sub>]<sub>2</sub> shows general structural features common to other bent zirconocene and  $\pi$ -arenechromium complexes but shows some unexpected features associated with the Zr-aryloxo bonding. Little evidence is found for either steric interactions between the ( $\eta$ -OC<sub>6</sub>H<sub>5</sub>)Cr(CO)<sub>3</sub> units or for Zr-O  $\pi$ -bonding. The O-arene bond does show a small degree of multiple-bond character, which is supported by the deviation of the O-C arene vector from the least-squares arene plane, suggesting that a small degree of a cyclohexadienone resonance form is contributing to Zr-arene bonding.

IT 117689-02-8P 117689-03-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

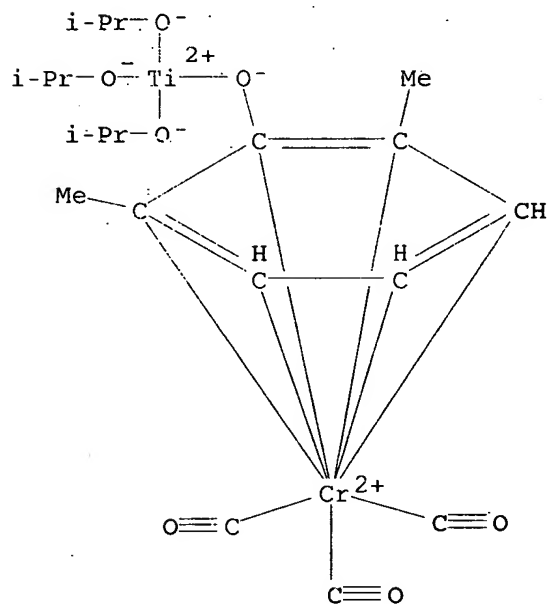
RN 117689-02-8 CAPLUS

CN Titanium, [ $\mu$ -( $\eta$ 6-phenolato-O)]tris(2-propanolato)(tricarbonylchromium) - (9CI) (CA INDEX NAME)



RN 117689-03-9 CAPLUS

CN Titanium, [ $\mu$ -[(1,2,3,4,5,6- $\eta$ )-2,6-dimethylphenolato-O]]tris(2-propanolato)(tricarbonylchromium) - (9CI) (CA INDEX NAME)



L6 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:631288 CAPLUS

DOCUMENT NUMBER: 109:231288

TITLE: Titanium and zirconium pyrophosphates and their uses

INVENTOR(S): Sugerman, Gerald; Monte, Salvatore Joseph

PATENT ASSIGNEE(S): Kenrich Petrochemicals, Inc., USA

SOURCE: Eur. Pat. Appl., 35 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

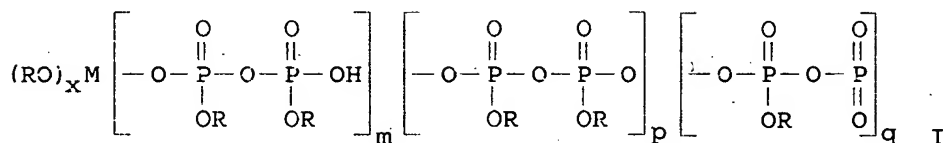
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

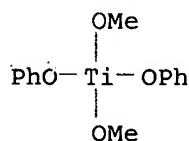
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 175542	A2	19860326	EP 1985-306445	19850911
EP 175542	A3	19871202		
EP 175542	B1	19931201		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4634785	A	19870106	US 1984-651119	19840914
ZA 8506754	A	19860430	ZA 1985-6754	19850903
IN 166752	A	19900714	IN 1985-DE725	19850903
AU 8547122	A1	19860320	AU 1985-47122	19850905
AU 575200	B2	19880721		
NO 8503548	A	19860317	NO 1985-3548	19850911
NO 165546	B	19901119		
NO 165546	C	19910227		
AT 97903	E	19931215	AT 1985-306445	19850911
JP 61118390	A2	19860605	JP 1985-203209	19850913
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CA 1240690	A1	19880816	CA 1985-490759	19850913
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GI

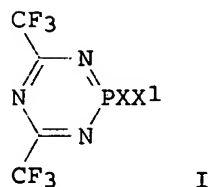


- AB Title compds. I (M = Zr, Ti; R = monovalent hydrocarbyl with halo or oxygen substituents; m = 0-4; x = 0-3; p = 0-2; q = 0-4, with provisos) are prepared by reaction of Ti or Zr tetraesters with P2O5 and organic hydroxy compds. For example, reaction of 1 mol each of P2O5 and Ti(OC8H17)4 in xylene at 35-95° gave 79% (C8H17O)2Ti[OP(O)(OC8H17)OP(O)(OC8H17)O]. Examples of I as flame retardants, adhesion promoters, and anticorrosive additives for solvent based acrylic-urethane primers are given.
- IT 116088-73-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with phosphorus pentoxide and alcs., pyrophosphates from)
- RN 116088-73-4 CAPLUS
- CN Titanium, dimethoxydiphenoxy-, (T-4)- (9CI) (CA INDEX NAME)



L5 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1988:423017 CAPLUS  
 DOCUMENT NUMBER: 109:23017  
 TITLE: Alkali triazaphosphininolates: synthesis and reactions  
 AUTHOR(S): Meyer, Matthias; Klingebiel, Uwe  
 CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Goettingen, Goettingen, 3400, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1988), 121(6), 1119-21  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 109:23017  
 GI



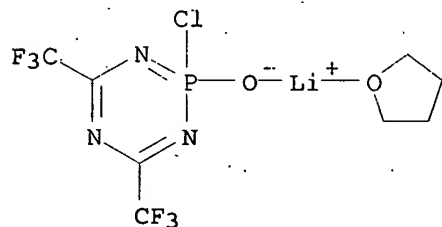
AB The alkali triazaphosphininolates I [X = OK (II), ONa (III), OLi (IV); X1 = F] are obtained from reaction of I (X = X1 = F, Cl) with NaOCHMe2, NaOCMe3, KOCHMe2, KOME3, and LiOSiMe3. The 2-fluorotriazaphosphininol I (X = OH, X1 = F) (V) is formed in the reaction of IV with HF. V reacts with KOH to yield II. The reaction of III with ClSiMe3 leads to the formation of the siloxytriazaphosphinine I (X = OSiMe3, X1 = F). I [X = NLiCMe3, NLiSiMe2CMe3 (VI); X1 = F] are obtained from the aminofunctional compds. and LiN(SiMe3)2. VI reacts with ClSiMe3 to give LiCl and I [X = N(SiMe3)(SiMe2CMe3), X1 = F].

IT 113035-93-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 113035-93-1 CAPLUS

CN Lithium, [2-chloro-2,2-dihydro-2-hydroxy-4,6-bis(trifluoromethyl)-1,3,5,2-triazaphosphorinato-O] (tetrahydrofuran)- (9CI) (CA INDEX NAME)

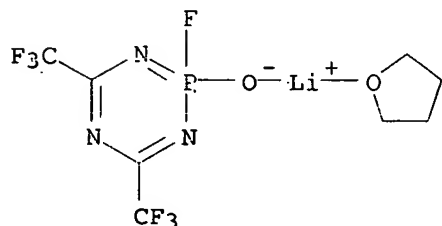


IT 113035-92-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, silylation and reaction of, with hydrogen fluoride)

RN 113035-92-0 CAPLUS

CN Lithium, [2-fluoro-2,2-dihydro-2-hydroxy-4,6-bis(trifluoromethyl)-1,3,5,2-triazaphosphorinato-O] (tetrahydrofuran)- (9CI) (CA INDEX NAME)



L6 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:637328 CAPLUS

DOCUMENT NUMBER: 107:237328

TITLE: Study of model esterifications and of polyesterifications catalyzed by various organometallic derivatives. I. Study of esterifications catalyzed by titanium derivatives  
AUTHOR(S): Leverd, Francois; Fradet, Alain; Marechal, Ernest  
CORPORATE SOURCE: Lab. Synth. Macromol., Univ. Pierre et Marie Curie, Paris, 75005, Fr.  
SOURCE: European Polymer Journal (1987), 23(9), 695-8  
CODEN: EUPJAG; ISSN: 0014-3057

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The efficiencies of several esterification catalysts were compared. The esterification of stearic acid by octadecanol catalyzed by organic Ti compds. was studied as a polyesterification model.  $\text{Ti}(\text{OBu})_4$  activity did not depend on initial acid concentration and remained unchanged during the reaction.

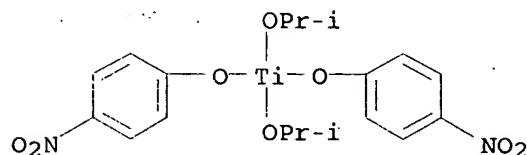
The catalysis was effective only when Ti ligands and alc. alkoxy groups could be exchanged; when this exchange was possible, the catalytic efficiency did not depend on the nature of the initial ligands provided that the alkoxy group was not too bulky.

IT 110448-08-3

RL: CAT (Catalyst use); USES (Uses)  
(catalysts, for esterification of stearic acid with octadecanol, as model for polyesterification)

RN 110448-08-3 CAPLUS

CN Titanium, bis(4-nitrophenolato-O1)bis(2-propanolato)-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:617078 CAPLUS

DOCUMENT NUMBER: 107:217078

TITLE: Formate esters by Cannizzaro-Tishchenko reaction of Grignard and sodium alkoxides with formaldehyde

AUTHOR(S): Bunce, Richard A.; Shellhammer, A. Joe, Jr.

CORPORATE SOURCE: Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078-0447, USA

SOURCE: Organic Preparations and Procedures International (1987), 19(2-3), 161-6

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:217078

AB Alkoxides  $\text{R1OM}(\text{R1} = \text{alkyl, cyclohexylmethyl, alkylcyclohexyl, Ph; M} = \text{MgBr, Na})$  were treated with  $\text{HCHO}$  to give the resp.  $\text{HCO}_2\text{R1}$ .

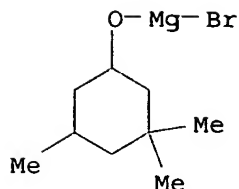
IT 111194-98-0 111194-99-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Cannizzaro-Tishchenko reaction of, with formaldehyde)

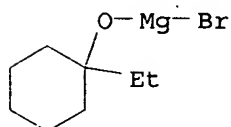
RN 111194-98-0 CAPLUS

CN Magnesium, bromo(3,3,5-trimethylcyclohexanolato)- (9CI) (CA INDEX NAME)





RN 111194-99-1 CAPLUS  
CN Magnesium, bromo(1-ethylcyclohexanolato)- (9CI) (CA INDEX NAME)



L6 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:478023 CAPLUS

DOCUMENT NUMBER: 107:78023

TITLE: Synthesis and structure of [(NMe<sub>2</sub>)<sub>3</sub>TiFe(CO)<sub>2</sub>(Cp)]: a stable iron-titanium bond

AUTHOR(S): Sartain, William J.; Selegue, John P.

CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY, 40506-0055, USA

SOURCE: Organometallics (1987), 6(8), 1812-15

CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:78023

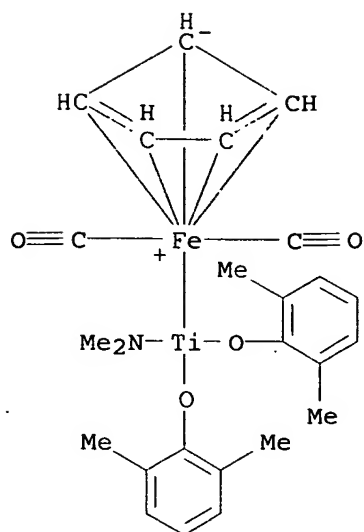
AB [Ti(NMe<sub>2</sub>)<sub>4</sub>] reacts with [FeH(CO)<sub>2</sub>(Cp)] (I; Cp = η<sup>5</sup>-cyclopentadienyl) to form [(Me<sub>2</sub>N)<sub>3</sub>TiFe(CO)<sub>2</sub>(Cp)] (II) by the elimination of 1 equiv of HNMe<sub>2</sub>. II was spectroscopically characterized, and its structure was determined by single-crystal x-ray diffraction. There is a direct, unsupported bond between Fe and Ti in II, with bond lengths of 2.566 (1) and 2.568 (1) Å in 2 independent mols. The relative orientation of the ligands on Fe and Ti suggests that there may be a π-component of the metal-metal bond. Amide Me groups distal to iron show unusually obtuse Ti-N-C angles of about 130°. Analogous complexes with **alkoxide** ligands on titanium are more labile than II. Reaction of II with [MoH(CO)<sub>3</sub>(Cp)] forms [(Me<sub>2</sub>N)<sub>2</sub>Ti{(μ-CO)Mo(CO)<sub>2</sub>(Cp)}<sub>2</sub>] and I.

IT 109284-62-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 109284-62-0 CAPLUS

CN Titanium, [dicarbonyl(η<sup>5</sup>-2,4-cyclopentadien-1-yl)iron]bis(2,6-dimethylphenolato)(N-methylmethanaminato)-, (Fe-Ti) (9CI) (CA INDEX NAME)

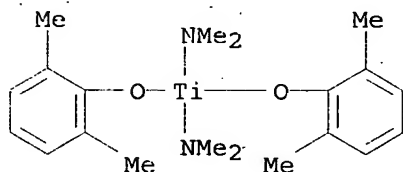


IT 109306-88-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with hydridoiron complex)

RN 109306-88-9 CAPLUS

CN Titanium, bis(2,6-dimethylphenolato)bis(N-methylmethanaminato)-, (T-4)-  
(9CI) (CA INDEX NAME)



L6 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:175925 CAPLUS

DOCUMENT NUMBER: 106:175925

TITLE: Reactions of anthrone with nontransition and transition metal alkoxides

AUTHOR(S): Tamano, Michiko; Koketsu, Jugo

CORPORATE SOURCE: Coll. Eng., Chubu Univ., Kasugai, 487, Japan

SOURCE: Nippon Kagaku Kaishi (1986), (6), 801-4

CODEN: NKAKB8; ISSN: 0369-4577

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 106:175925

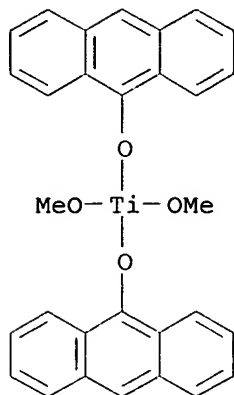
AB The reactions of anthrone with group B metal alkoxides (RO)4M (R = alkyl, M = Ge and Sn) at 140°C for a week provided 10-alkylanthrone, which were considered to be rearrangement products from the substituted intermediates: dialkoxybis(9-anthryloxy)metals. Group IVA and VA metal alkoxides (RO)4M (M = Ti and Zr), OV(OR)3 and (RO)5Nb reacted with anthrone at 140°C for 24 h to give the substituted intermediates. These unstable intermediates decomposed giving anthracene and 9,10-dihydroanthracene. In these cases, Meerwein type reduction of 9-anthryloxy group might provide anthracene, and following reduction of anthracene gave 9,10-dihydroanthracene.

IT 107931-49-7P

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, from reaction of anthrone with tetraalkoxytitanium)

RN 107931-49-7 CAPLUS

CN Titanium, bis(9-anthracenolato)dimethoxy-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:4367 CAPLUS

DOCUMENT NUMBER: 106:4367

TITLE: The role of early transition metal azides as catalysts of the ring-opening reaction of epoxides with trimethylsilyl azide

AUTHOR(S): Blandy, Claudine; Gervais, Daniele; Cardenas, Maribel Suarez

CORPORATE SOURCE: Lab. Chim. Coord., Univ. Paul Sabatier, Toulouse, 31 400, Fr.

SOURCE: Journal of Molecular Catalysis (1986), 34(1), 39-46  
CODEN: JMCADS; ISSN: 0304-5102

DOCUMENT TYPE: Journal

LANGUAGE: English

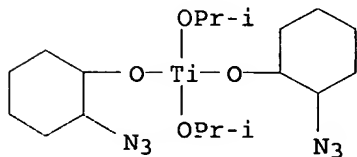
AB Complexes of early transition metals (titanium, vanadium, ...) catalyze the reaction of epoxides with  $\text{Me}_3\text{SiN}_3$ . When an azido complex is used as precursor, the reaction follows an overall second-order law and the rate constant is proportional to the complex concentration. The regioselectivity ( $\alpha$ - or  $\beta$ -cleavage of the ring) is compared to that of the stoichiometric reaction of the transition metal azide with epoxides. The catalytic mechanism involves the intermediary formation of a complex resulting from the nucleophilic attack of the epoxide ring by the  $\text{N}_3$  group bonded to the transition metal atom.

IT 105334-45-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 105334-45-0 CAPLUS

CN Titanium, bis(2-azidocyclohexanolato-O)bis(2-propanolato)-, [T-4-(trans)-(trans)]- (9CI) (CA INDEX NAME)



L6 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:479892 CAPLUS

DOCUMENT NUMBER: 105:79892

TITLE: Neoalkoxy organotitanates and organozirconates useful  
 as coupling and polymer processing agents  
 INVENTOR(S): Sugerman, Gerald; Monte, Salvatore J.  
 PATENT ASSIGNEE(S): Kenrich Petrochemicals, Inc., USA  
 SOURCE: Eur. Pat. Appl., 56 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 164227	A2	19851211	EP 1985-303352	19850513
EP 164227	A3	19870902		
EP 164227	B1	19900816		
R: BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4600789	A	19860715	US 1984-609727	19840514
US 4623738	A	19861118	US 1985-725437	19850422
NO 8501845	A	19851115	NO 1985-1845	19850509
NO 167393	B	19910722		
NO 167393	C	19911030		
ZA 8503532	A	19861230	ZA 1985-3532	19850509
IN 170651	A	19920502	IN 1985-DE389	19850509
CA 1237140	A1	19880524	CA 1985-481428	19850513
AU 8542475	A1	19851121	AU 1985-42475	19850514
AU 575165	B2	19880721		
JP 61022093	A2	19860130	JP 1985-102527	19850514
JP 03080159	B4	19911224		
CN 85104987	A	19861119	CN 1985-104987	19850701
CN 1005712	B	19891108		
IN 170585	A	19920418	IN 1987-DE1123	19871223
JP 02138285	A2	19900528	JP 1989-238325	19890913
JP 06000791	B4	19940105		
JP 05339421	A2	19931221	JP 1991-226650	19910318
JP 08034745	B4	19960329		

PRIORITY APPLN. INFO.:

US 1984-609727	A	19840514
US 1985-725437	A	19850422
US 1984-651119	A2	19840914
IN 1985-DE389	A	19850509

AB A neoalkoxy compound RCR1R2CH2OMAaBbCc (M = Ti or Zr; each R, R1, and R2 = C1-20 hydrocarbyl, optionally halo- or ether-substituted, and R2 may also be an oxy or ether-substituted oxy derivative; each A, B, and C = monovalent aryloxy, thioaryloxy, diester phosphate or pyrophosphate, oxyalkylamino, sulfonyl, or carboxyl; a + b + c = 3) has good thermal and solvolytic stability, is useful for compounding with polymers at high temps. (>200°), and is also useful in peroxide-cured or air-cured polymerization systems for coupling fillers to polymer and, in some cases, accelerating the polymerization. Thus, 1 mol TiCl4 was added to a xylene solution of 1 mol Me3CCH2OH and 3 mol HOP(O)(OC8H17)2 during 2 h at 45-60° in N and kept for an addnl. 2 h. The mixture was heated in vacuo to evaporate the solvent, giving Me3CCH2OTi[OP(O)(OC8H17)2]3 (I) (87% yield). The compound had solvolysis resistance in BuOH (time required for disappearance of 50% solute at 25°) 48 h, vs. 0.1 h for Me2CHOTi[OP(O)(OC8H17)2]3 (II). A composition comprising ABS resin 59.8, talc 40.0, and 65:35 I-silica powder mixture 0.2% was injection molded at 230° to give a molding having tensile strength 42 MPa, elongation 35%, flexural strength 78 MPa, flexural modulus 2.4 GPa, and notched Izod impact strength 0.4 kJ/m, vs. 37, 28, 70, 2.2, and 0.3, resp., for a composition prepared with II instead of

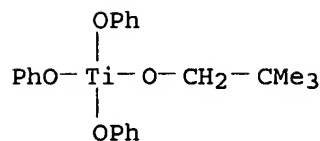
I.

IT 103245-61-0P

RL: PREP (Preparation)

(preparation of heat- and solvolysis-resistant, as coupling and polymer processing agents)

RN 103245-61-0 CAPLUS  
 CN Titanium, (2,2-dimethyl-1-propanolato)triphenoxy-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:19382 CAPLUS

DOCUMENT NUMBER: 104:19382

TITLE: Enantioselective addition of aryl groups to aromatic aldehydes using chiral aryltitanium binaphthol derivatives

AUTHOR(S): Seebach, Dieter; Beck, Albert K.; Roggo, Silvio; Wonnacott, Anne

CORPORATE SOURCE: Lab. Org. Chem., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.

SOURCE: Chemische Berichte (1985), 118(9), 3673-82  
 CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 104:19382

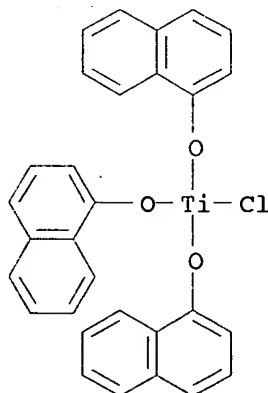
AB Chiral, nonracemic organotitanium reagents were generated in situ from binaphthol,  $\text{ClTi}(\text{CHMe}_2)_3$ , and aryl Grignard reagents in THF. These reagents transfer aryl groups to aromatic aldehydes to afford carbinols (e.g.,  $\text{PhCHROH}$ , where R = tolyl, naphthyl, 1-pyrenyl, etc.) with high enantioselectivity. In cases where the absolute configuration of the products is known, the reaction occurs with relative topicity 1K.

IT 88759-75-5 95045-75-3 99412-42-7  
 99412-43-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (complexation of, with binaphthol)

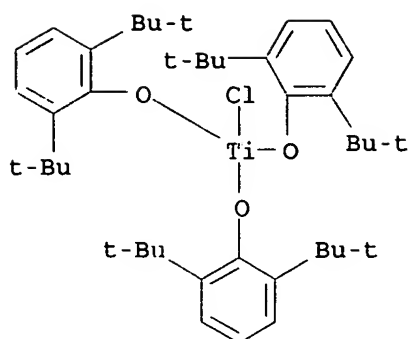
RN 88759-75-5 CAPLUS

CN Titanium, chlorotris(1-naphthalenolato)-, (T-4)- (9CI) (CA INDEX NAME)

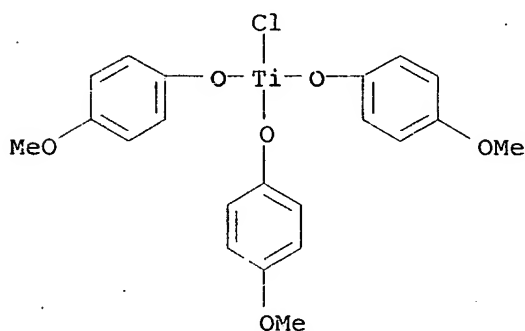


RN 95045-75-3 CAPLUS

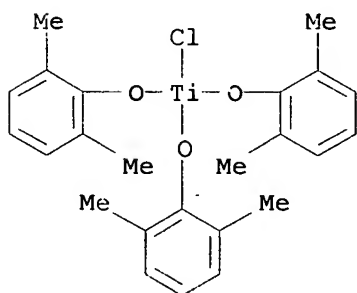
CN Titanium, tris[2,6-bis(1,1-dimethylethyl)phenolato]chloro-, (T-4)- (9CI) (CA INDEX NAME)



RN 99412-42-7 CAPLUS  
 CN Titanium, chlorotris(4-methoxyphenolato-O1)-, (T-4)- (9CI) (CA INDEX NAME)



RN 99412-43-8 CAPLUS  
 CN Titanium, chlorotris(2,6-dimethylphenolato)-, (T-4)- (9CI) (CA INDEX NAME)



L6 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1985:596194 CAPLUS

DOCUMENT NUMBER: 103:196194

TITLE: Multiple metal-carbon bonds. 38. Preparation of trialkoxymolybdenum(VI) alkylidyne complexes, their reactions with acetylenes, and the x-ray structure of  $\text{Mo}[\text{C}3(\text{CMe}_3)_2][\text{OCH}(\text{CF}_3)_2](\text{C}_5\text{H}_5\text{N})_2$

AUTHOR(S): McCullough, Laughlin G.; Schrock, Richard R.; Dewan, John C.; Murdzek, John C.

CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (1985),

107(21), 5987-98  
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 103:196194

GI For diagram(s), see printed CA Issue.

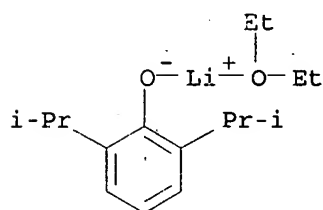
AB MoRNpn3 (I; R = .tplbond.CCMe3, throughout; Npn = CH2CMe3) was prepared in .apprx.35% on a multigram scale by adding MoO2Cl2 in THF to 6 equiv of NpnMgCl in Et2O. MoRX3(dme) (X = Cl, Br; dme = MeOCH2CH2OMe) were prepared by treating I with 3 equivalent of HX in the presence of dme. MoRCl3(dme) reacted with alkoxide salts to give MoR(OR1)3 [R1 = CMe3, CHMe2, CH2CMe3, CMe2CF3, CMe(CF3)2, C6H3(CHMe2)2-2,6 (II)], MoR(OR2)3(dme) [R2 = CH(CF3)2, CMe(CF3)2, C(CF3)3], or MoR(OR2)2Cl(dme). Internal acetylenes such as R3C.tplbond.CR3 (R3 = Me, Et, Pr, Ph) reacted smoothly with II and all fluoroalkoxide complexes, to give new alkylidyne complexes Mo(.tplbond.CR3)(OR4)3 or Mo(.tplbond.CR3)(OR4)3(dme) [R4 = CMe2CF3, CMe(CF3)2, CH(CF3)2, C6H3(CHMe2)2-2,6]. Terminal acetylenes R5C.tplbond.CH (R5 = CHMe2, Pr, Ph) reacted with MoR(OCMe3)3 to produce Me3CC.tplbond.CH and Mo(.tplbond.CR5)(OCMe3)3. Reactions between terminal acetylenes R5C.tplbond.CH (R5 = CMe3, Ph, CHMe2) and fluoroalkoxide complexes gave deprotio molybdenacyclobutadiene complexes Mo(C3R52)(OR2)2 (R2 = initial R2), some of which can be isolated only as bis ligand adducts, Mo(C3R52)(OR2)2L2 (III; L = py, dme). The x-ray crystal structure of III [R2 = CH(CF3)2; R5 = CMe3; L = py] (IV) showed it is a pseudotetrahedron with the py ligand trans to a planar MoC3 ring. The 2 O atoms of the OCH(CF3)2 ligands are bent away from the ring system and the  $\alpha$ -CMe3 groups are bent away from Mo. MoR(OR2)3(dme) [R2 = CMe(CF3)2, C(CF3)3, C6H3(CHMe2)2-2,6] are excellent catalysts for the metathesis of 3-heptyne.

IT 98193-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with molybdenum neopentylidyne chloro complex)

RN 98193-96-5 CAPLUS

CN Lithium, [2,6-bis(1-methylethyl)phenolato][1,1'-oxybis(ethane)]- (9CI);  
(CA INDEX NAME)



L6 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1963:81508 CAPLUS

DOCUMENT NUMBER: 58:81508

ORIGINAL REFERENCE NO.: 58:13945e-h

TITLE: Heterocyclic syntheses with malonyl chloride. VII.  
Dihydropyrano[3,4-e]-1,3-oxazines from isocyanates,  
and their degradation to dihydro-2,4-dioxo-1,3-  
oxazines and thence conversion into pyridones

AUTHOR(S): Butt, M. Aslam; Elvidge, J. A.; Foster, Arthur Brian

CORPORATE SOURCE: Imp. Coll. Sci. Technol., London

SOURCE: Journal of the Chemical Society, Abstracts (1963)  
3069-81

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 58:81508

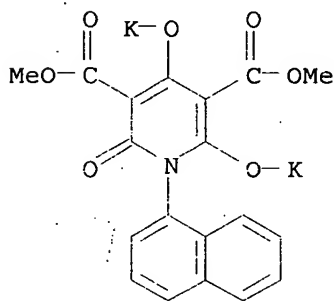
GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 12476e. Isocyanates with malonyl chloride yield 3-substituted 7-chloro-3,4-dihydro-2,4,5-trioxo-2H,5H-pyrano[3,4-e]-1,3-oxazines (I, X = O). Phenyl isothiocyanate yields the 4,5-dioxo-3-phenyl-2-thio compound (I, R = Ph, X = S). Alcs. (R'OH) open the chloropyrone ring of the new bicyclic compds. (I, X = O) and give derivs. of 3,4-dihydro-2,4-dioxo-2H-1,3-oxazine (II). These are isomerizable by alkoxide to 1-substituted dialkyl 1,2-dihydro-4,6-dihydroxy-2-oxopyridine-3,5-dicarboxylates (III), but aqs. alkali yields the corresponding 3-monoesters II react further with alc. to give diester anilides of acetone-1,1,3-tricarboxylic acid, R'O<sub>2</sub>CCH<sub>2</sub>C(OR'):C(CO<sub>2</sub>R')CONHPh and R'O<sub>2</sub>CCH<sub>2</sub>C(OH):C(CO<sub>2</sub>R')CONHPh, which are cyclized by alkali to hydroxypyridones. The 4,6-dihydroxypyridone ester IV was converted into the 4,6-dichloropyridone ester and thence by alkaline hydrogenolysis into 1-phenylpiperidone. Ultraviolet and infrared absorptions and proton magnetic resonance results provided information about the fine structures of some of these potentially tautomeric compds.

IT 95024-20-7, Potassium, [[3,5-dicarboxy-1,6-dihydro-1-(1-naphthyl)-6-oxo-2,4-pyridinediyl]dioxy]di-, dimethyl ester (preparation of)

RN 95024-20-7 CAPLUS

CN Potassium, [[3,5-dicarboxy-1,6-dihydro-1-(1-naphthyl)-6-oxo-2,4-pyridinediyl]dioxy]di-, dimethyl ester (7CI) (CA INDEX NAME)



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